Multiscale Strength Homogenization – Application to Shale Nanoindentation

by

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Abstract

Shales are one of the most encountered materials in sedimentary basins. Because of their highly heterogeneous nature, their strength prediction for oil and gas exploitation engineering has long time been an enigma. In this thesis, we propose a two-scale non-linear procedure for the homogenization of their yield design strength properties, based on the Linear Comparison Composite Theory. At Level 0, the intrinsic friction of shales is captured via a cohesive-frictional strength criterion for the clay particles (Drucker-Prager). Level I is composed of a porous clay phase and Level II incorporates silt and quartz grains. Homogenization yields either an elliptical or an hyperbolic strength criterion, depending on the packing density of the porous clay phase. These criteria are employed in an original reverse algorithm of indentation hardness to develop hardness-packing density scaling relations that allow a separation of constituent properties and volume fraction and morphology parameters, including interface conditions between the porous clay matrix and the (rigid) silt inclusions. The application of this algorithm to 11 shale samples from the GeoGenome project data base allows us to identify: (i) an invariant value of the solid hardness of clay particles, which is independent of clay mineralogy, porosity, etc.; and (ii) shale independent scaling relations of the cohesion and of the friction coefficient with the mean clay packing density, which provides some evidence that the elementary building block of shale is a clay polycrystal. The use of these scaling relations in the Level II-homogenization provides a first-order model for the prediction of the macroscopic strength properties of shale, based on only two parameters that delineate shale’s macroscopic diversity: clay packing density and silt inclusion volume fraction.

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Part I

General Presentation
Chapter 1

Introduction

1.1 Industrial Context

The strength properties of shale, the sealing formation in most hydrocarbon reservoirs, are of critical importance for many fields of oil and gas exploitation engineering, ranging from hydraulic fracturing and well bore stability to the appropriate choice of the drilling fluid chemistry and density and unwanted sand production. Shales are made of highly compacted clay particles of sub-micrometer size, nanometric porosity and different mineralogy. Clayish sediments are the start and end point of hydrocarbon migration: hydrocarbons originate from their organic content and are trapped by their low permeability. Measuring and predicting the strength properties is of utmost importance. Classically, strength properties are estimated using macroscopic triaxial testing methods. However, this classical technique requires expensive macroscopic material sampling often from very high depths. Furthermore, shales exhibit a high degree of heterogeneity, which makes it difficult to extrapolate from one sample to another. The current limitations in knowledge of shale strength behavior frequently result in wellbore instability, that cost the oil and gas industry approximately $6 billions a year [110].

Recently, a new approach has been suggested to deal with the intrinsic diversity of earth materials. Coined the GeoGenome project [1], [112], this approach aims at identifying a fundamental unit of material invariant behavior of sedimentary rocks. Once this scale is identified, it is possible to upscale the intrinsic material behavior from the nanoscale to the macroscale, and quantify macroscopic diversity on the basis of a few material invariant properties.
The work presented in this thesis is part of this 'genoming' effort of geomaterials, and presents a literal dive down to the nanoscopic scale, in search of elementary strength properties, followed by a two-steps ascent to the scale of day-to-day engineering applications of shale.

1.2 Research Objectives and Approach

Shale is probably one of the most complicated and intriguing natural material present on earth. The multiphase composition is permanently evolving over various scales of length and time, creating in the course of this process the most heterogeneous class of material in existence. Shale is a multiscale heterogeneous material (Figure 1-1). It is composed of elementary clay particles (Kaolinite, Smectite, Illite, etc...) forming a porous clay composite material at the micrometer scale. At a scale above, this textured clay composite is intermixed with silt and quartz grains of micrometer size. Finally, heterogeneities are also observed at the macroscale where layers are deposited along with detrital grains.

The overall objective of this thesis is the strength prediction of shale macroscopic strength behavior. In order to reach our goal, we break down the problem into three different tasks.

1. The first task consists in developing a micromechanics model for strength properties of shale, which must be sufficiently flexible to account for the characteristic heterogeneities of shale materials, namely the clay porosity and the silt inclusions, which manifest themselves at two different scales. The approach which we choose here is based on nonlinear homogenization theory, which is applied to shale's multiscale structure: We assume the existence of an elementary clay building block (Level '0' in Fig. 1-1). A first homogenization step yields the strength domain of the porous clay phase (Level '1' in Fig. 1-1), viewed as a cohesive-frictional porous material. A second homogenization step adds silt inclusions to the porous clay phase to yield the macroscopic strength response.

2. The second task consists in calibrating the model. In view of the GeoGenome approach, calibration means here to separate constituent properties of the solid phases from volume fractions and morphology parameters. To this end, we will make use of nanoindentation results of shales. Nanoindentation has provided the materials science community with a versatile tool to probe material volumes, that cannot be recapitulated in bulk form
Figure 1-1: Multiscale structure thought model of shale (adapted from [77])
for macroscopic testing. Nanoindentation on shales is able to test the porous clay phase [101],[102],[10]. The second task thus consists in developing an indentation analysis that allows separating the constituent strength properties of the solid clay phase from volume fractions and morphology parameters.

3. Validation of this approach for shales is the third task. This will be achieved by applying the developed indentation analysis tools to nanoindentation results of shales of different mineralogy, bulk density and porosity. We will make use of the GeoGenome database of eleven different shale materials. The aim of this task is to identify universal strength-microstructure relations that hold for any shale material. Finally, by using these relations in the multiscale strength model of shale, macroscopic strength prediction should be possible.

1.3 Thesis Outline

This report is divided into four parts:

Following this introduction, Part II of this thesis deals with strength homogenization. It is composed of two chapters: Chapter 2 provides an overview of strength homogenization methods based on yield design theory. Among those methods, the Linear Comparison Composite Theory proposed by Castañeda [80], [81],[83] appears to us most suited for our purpose, which is the strength homogenization of strength properties of multiscale heterogeneous materials. This is shown in Chapter 3 in the original development of a two-scale micromechanics model for shale: At the scale of the porous clay composite of shale (Level 'I' in Fig. 1-1), we derive the strength domain of a composite composed of a cohesive-frictional solid and pores, which leads to an elliptical or a hyperbolic strength criterion. Then, in a second homogenization step (Level 'II' in Fig. 1-1), we homogenize the strength behavior of the porous clay and rigid inclusions (with and without adhesion) to obtain an estimate of shale macroscopic strength behavior.

Part III is devoted to the indentation analysis of the strength properties of the constituents of an heterogeneous material obtained from indentation hardness measurements at the scale of the composite. It is composed of two chapters. Chapter 4 provides a brief introduction to the indentation technique and indentation analysis. It focusses in particular on the self-similarity
of the indentation test, the extraction of the indentation modulus and the indentation hardness from an indentation test, and on a dimensional analysis of the relevant quantities involved in an indentation in an heterogeneous material, which at a scale smaller than the indentation depth is composed of different phases. This is the situation we consider in Chapter 5, in which we use the expressions of the homogenized strength criteria derived in Chapter 3 for indentation analysis. In fact, by simulating the indentation experiment in this homogenized medium, hardness-packing density scaling relations are derived which make the link between the strength properties of the constituents, morphology parameters and hardness as measured in an indentation test.

Part IV deals with the application of the tools developed throughout this thesis to shales. In particular, in order to employ the hardness-microstructure relations developed in Part III, Chapter 6 presents an original algorithm for the reverse analysis of the packing density distribution and particle properties from nanoindentation data. Chapter 7 applies this algorithm to a large range of shale materials of different geographical origins, mineralogy, density, porosity, etc. Finally, in the light of the results obtained at the nanoscale, we discuss the macroscopic strength domain of shales using the homogenization relations derived in Part II.

The main findings and contributions of this study are summarized in Chapter 8, which also suggests perspectives for future research.

1.4 Research Significance

The research presented in this thesis aims at contributing to the GeoGenome project, by providing a first micromechanics-based model for the strength prediction of shale.

The prime challenge in this development is to capture the observed macroscopic variability of shale strength properties through a handful of easily identifiable and varying parameters, and to relate these parameters as much as possible to mineralogy data, that one can extract from seismic logs, drilling fluid composition, depth, pore pressure and other available geological information. Such a reductionist approach requires the use of micromechanics models, which by construction are reductionist. In this regard, this work follows in the footsteps of several investigations that deal primarily with the homogenization of elastic and poroelastic properties
of shales [33],[100],[77], and extends these approaches to strength properties of shales.

From a mechanics point of view, the second challenge of this study is to identify and apply the appropriate homogenization method for strength properties of shales. As regards the porous clay phase, this work is inspired by the strength homogenization models for cohesive-frictional porous composites developed by Dormieux and co-worker [3],[5],[38]. Yet, with the focus on a two-scale upscaling model required for shales, a more general and flexible approach is required. For this reason we resort to the Linear Comparison Composite Theory of Castañeda [80],[81],[83], which we put to work for the multiscale homogenization of strength properties of shale.

From an indentation analysis point of view, the third challenge is to link indentation data to meaningful mechanical properties. In this regard, this work follows in the footstep of previous investigations of hardness–strength property–microstructure relations of cohesive-frictional materials [44],[45] and cohesive-frictional porous materials [19],[20], and makes extensive use of the GeoGenome shale nanoindentation data base generated by C. Bobko at MIT [10].

As such, the tools developed in this thesis contribute to the implementation, for sedimentary rocks, of the materials science paradigm between nano- and microstructure, constituent properties and macroscopic performance. It is on this basis that we expect progress in nanoscience and nanoengineering to impact everyday engineering application and society.
Part II

Strength Homogenization
Chapter 2

Elements of Strength Homogenization

The development of a predictive model for strength of shales will make extensive use of the theory of strength homogenization. In contrast to the homogenization of elasticity properties, which can make use of linear homogenization theory, as summarized in the Appendix A of this report, strength homogenization refers to an intrinsically nonlinear phenomenon, requiring the use of recent advances in nonlinear homogenization theory. The application of nonlinear homogenization theory to shales is in short the focus of this first part. In particular, this Chapter sets the stage by reviewing key elements of strength homogenization, based primarily on the scholarly contributions by Castañeda [80], [81],[83], Suquet [95] [93] [94], and Dormieux and co-worker [37] [3] [4]. The next Chapter will show the application of these elements to the multiscale microstructure of shale.

2.1 Problem Formulation

The goal of strength homogenization is to derive the macroscopic strength domain of a heterogeneous material from the knowledge of the microscopic strength domains of the different materials that make up the composite material. The most common mechanical system of investigation is a representative volume element (RVE) of a heterogeneous material. The RVE is subjected at its boundary oriented by the outward unit normal \( n(x) \) to a regular traction
condition:
\[ \forall \mathbf{x} \in \partial V : \mathbf{t}(\mathbf{x}) = \mathbf{\Sigma} \cdot \mathbf{n}(\mathbf{x}) \]  

(2.1)

where \( \mathbf{\Sigma} \) is the macroscopic stress tensor, which is the volume average of the microscopic stress field \( \mathbf{\sigma}(\mathbf{x}) \) over the REV:

\[ \mathbf{\Sigma} = \frac{1}{|V|} \int_V \mathbf{\sigma}(\mathbf{x}) \, dV = \bar{\mathbf{\sigma}}(\mathbf{x}) \]  

(2.2)

2.1.1 Yield Design Theory

The mechanics theory the most appropriate for strength upscaling is yield design theory. Yield design theory deals with the plastic collapse of a material system or structure, and explores the following two complementary key ideas [30] [65] [86]:

1. Plastic collapse occurs once the structure has exhausted its capacity to develop, in response to a prescribed loading, stress fields which are statically compatible with the external loading, and plastically admissible with the strength of the constitutive material. The capacity is thus exhausted to sustain any additional load by means of stresses in the structure, which satisfy equilibrium and which do not exceed the local material strength.

2. Plastic collapse occurs when the work rate supplied from the outside can no more be stored as recoverable (free) energy into the system. As a consequence, this work rate is entirely dissipated into heat form. The material, during plastic collapse, locally dissipates the externally applied work at the highest possible rate. Any additional supplied work is dissipated through plastic yielding in the material bulk and/or along narrow bands of surfaces of discontinuity.

As shown here below, these two key ideas define one and the same, that is the strength domain of the material.

2.1.2 Stress-Strength Approach

Consider first the stress-strength approach of yield design applied to the RVE. The problem to be solved consists of finding stress fields \( \mathbf{\sigma}^*(\mathbf{x}) \) that are both statically admissible and compatible with the strength domain of the heterogeneous material. In particular, let \( S(\mathbf{\Sigma}) \) be
the set of statically admissible stress fields for the macroscopic stress $\Sigma$ applied at the boundary, according to (2.1):

$$S(\Sigma) = \{ \sigma^* (x), \ \text{div} \sigma^* (x) = 0 \ \text{in} \ V \ \text{and} \ t = \Sigma \cdot n \ \text{on} \ \partial V \} \ \ (2.3)$$

Furthermore, let $\mathcal{R}$ be the set of strength compatible (or plastically admissible) stress fields:

$$\mathcal{R} = \{ \sigma^* (x), \ \forall x \in V \ \ \sigma^* (x) \in G (x) \} \ \ (2.4)$$

where $G (x)$ is the local strength domain of the material (see Table 2.1), which is assumed to be bounded and strictly convex, as expressed by a strictly convex function $f(\sigma)$, such that:

$$G = \{ \sigma | f(\sigma) \leq 0 \} \ \ (2.5)$$

It is then readily understood that a combination of (2.3) and (2.4) yields a definition of the set of potentially sustainable macroscopic stresses $\tilde{G}$:

$$\tilde{G} = \{ \Sigma^* | \exists \sigma^* (x), \ \sigma^* (x) \in S(\Sigma^*) \ \text{and} \ \sigma^* (x) \in \mathcal{R} \} \ \ (2.6)$$

This set does not necessarily coincide with the set of the maximum stresses that the structure can actually sustain, which we will denote by $G^{\text{hom}}$. In return, the set $\tilde{G}$ includes $G^{\text{hom}}$, but it may as well include macroscopic stresses that are potentially sustained, but not actually supported. Otherwise said, without any further consideration, any stress that does not belong to $\tilde{G}$ will not be sustained.

### 2.1.3 Dual Approach: Maximum Plastic Dissipation Capacity

There exists a dual approach to define the strength of a material within the context of yield design theory. It is based on the premise that the material, at plastic collapse, has exhausted its capacity to store the external work rate into recoverable elastic energy. As a consequence it is entirely dissipated into heat form. The external work rate supplied to the RVE is obtained
The strength of a material refers to its ability to sustain an applied force. As this ability is not infinite, the strength criterion characterizes the maximum sustainable stress. Strength is a priori independent of the elastic deformation the material may have undergone until it reaches its actual maximal bearable load. For instance, during a tensile test, following elastic and eventually plastic deformation, the material will fail at a maximum load. The stress, \( \sigma_{\text{max}} \), associated with this maximum load, is the maximum sustainable stress.

The extension of this 1-D situation to any kind of loading leads to defining the strength domain of a material. Indeed, consider a progressive loading of the form \( \sigma = \lambda \sigma_0 \), with \( \sigma_0 \) a reference stress state generated by loading, and \( \lambda \) a scalar loading parameter. As long as \( \lambda \) is small enough, the material can support \( \sigma \). Then, \( \lambda \) is increased until it reaches a maximal possible value, which defines the maximal stress, \( \sigma_{\text{max}} \), corresponding to the load case \( \sigma_0 \). By repeating this experiment for all possible load cases, the domain of admissible stresses, \( G \), is found.

Table 2.1: Background: Strength and Strength Domain.

from an application of the Hill Lemma for the boundary condition (2.1):

\[
\delta W = \frac{1}{|V|} \int_{\partial V} t(\bar{x}) \cdot \mathbf{v}^*(\bar{x}) \, da = \sigma(\bar{x}) : \mathbf{d}(\bar{x}) = \Sigma : \mathbf{D}
\]

(2.7)

where \( \mathbf{D} \) and \( \mathbf{d}(\mathbf{v}^*(\bar{x})) = \frac{1}{2} (\nabla \mathbf{v}^* + (\nabla \mathbf{v}^*)^T) \) are respectively the macroscopic and the microscopic strain rate field that relate to the microscopic velocity field \( \mathbf{v}^*(\bar{x}) \) by:

\[
\mathbf{D} = \mathbf{d}(\bar{x}) = \frac{1}{2|V|} \int_{\partial V} (\mathbf{v}^* \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{v}^*) \, da
\]

(2.8)

The velocity field \( \mathbf{v}^* \) is kinematically admissible in the sense of yield design theory: since plastic collapse cannot be prescribed by constraining the velocity to non-zero values, all what \( \mathbf{v}^* \) needs to satisfy are zero-velocity boundary conditions. Given the regular stress boundary condition (2.1), there are, therefore, no a-priori restrictions on the velocity field \( \mathbf{v}^* \).

On the other hand, the only restriction on the dissipated work rate is that it must be finite; which is due to the fact that the material cannot sustain locally infinite stresses. This leads to introducing the support function \( \pi(d) \) as the maximal possible value of the locally dissipated
Figure 2-1: Associated flow rule: the strain rate is normal to the surface $\partial G$.

work rate or maximum dissipation capacity of the material:

$$\pi (d) = \sup_{\sigma^* \in G} \sigma^* : d$$  \hspace{1cm} (2.9)

It is then possible to show that if $\sigma$ is the stress on the boundary of $G$ maximizing the work rate (i.e. $\sigma : d = \pi (d)$), then $\sigma$ and $d$ are linked by:

$$\sigma = \frac{\partial \pi}{\partial d} (d)$$ \hspace{1cm} (2.10)

Figure 2-1 illustrates this result: the strain rate associated with a given stress on the boundary of the strength domain $G$ is normal to the surface $\partial G$ of this strength domain.

An important feature of the support function $\pi$ is that it is homogeneous, of degree 1. Indeed, from its definition (2.9) and by linearity of the tensor product, it has the following property:

$$\pi (\lambda d) = \sup_{\sigma \in G(x)} \sigma : (\lambda d) = \lambda \sup_{\sigma \in G(x)} \sigma : d = \lambda \pi (d)$$ \hspace{1cm} (2.11)

In addition, differentiating with respect to $\lambda$ yields:

$$\frac{\partial \pi}{\partial d} (\lambda d) = \frac{\partial \pi}{\partial d} (d)$$ \hspace{1cm} (2.12)
Relation (2.12) means that if a stress on the boundary $\partial G$ of the strength domain $G$ is associated with a given strain rate $d_0$ then it is associated with every strain rate collinear to $d_0$. These two properties will often be used throughout the forthcoming derivations.

Definition (2.9) constitutes an alternative way of defining the local strength domain of materials based on their dissipation capacity. We are left with applying this dual definition to the homogenization problem of the RVE. To this end, recall that the stress field $\sigma^*$ in definition (2.9) of the support function $\pi$, belongs to $G(x)$ at any point $x$. It follows:

$$\forall x \in \Omega \quad \sigma^* : d(y^*) \leq \pi(d(y^*), x) \quad (2.13)$$

Then, substituting (2.13) in (2.7) yields:

$$\delta W(\sigma^*, y^*) = \Sigma : D \leq \pi(d(y^*), \overline{x}) \quad (2.14)$$

Equation (2.14) is an alternative way to characterize macroscopic stresses that can potentially be sustained by the material-structure. Indeed, for a given kinematically admissible velocity field $v^*$, we can define the set $E(y^*)$ of macroscopic stresses that do not violate relation (2.14):

$$E(y^*) = \left\{ \Sigma^* | \exists \sigma^*(x), \sigma^*(x) \in S(\Sigma^*) \text{ and } \delta W(\sigma^*, y^*) = \Sigma^* : D \leq \pi(d(y^*), \overline{x}) \right\} \quad (2.15)$$

If we select only stresses that are not "eliminated" by any velocity field, we end up with a kinematical version of the set of potentially supportable macroscopic stresses $\tilde{G}_K$:

$$\tilde{G}_K = \bigcap_{y^*} E(y^*) \quad (2.16)$$

Since every stress in $\tilde{G}$ respects condition (2.13), it belongs to $\tilde{G}_K$; that is, $\tilde{G} \subset \tilde{G}_K$. However, it is possible to show [86] that, under some mathematical assumptions, these two sets are equal:

$$\tilde{G} = \tilde{G}_K \quad (2.17)$$

In other words, $\tilde{G}_K$ is the dual form of $\tilde{G}$, and thus it is bounded and convex.

It is worthwhile to have a second look on the infinite intersection (2.16) and on the inequality.
\[ \Sigma^* : D \leq \pi (d(v^*), \bar{x}) \] in (2.15). In particular, consider an element \( \Sigma \) at the boundary of \( \tilde{G} \). If the term \( \Sigma : D \) was strictly smaller\(^1\) than \( \pi (d(v^*), \bar{x}) \) for any kinematically admissible velocity field \( v^* \), then, by linearity, a stress \((1 + \epsilon) \Sigma \) just a little greater than \( \Sigma \), would respect \((1 + \epsilon) \Sigma : D \leq \pi (d(v^*), \bar{x}) \) for any \( v^* \); and hence would be within \( \tilde{G} \), which clearly contradicts the fact that \( \Sigma \) is at the boundary of \( \tilde{G} \). This illustrates that for an element \( \Sigma \) at the boundary of \( \tilde{G} \), there exists a velocity field \( v^* \) that saturates the inequality. We will assume that we have found a macroscopic stress \( \Sigma \) with its microscopic stress field \( \sigma (x) \) and a velocity field \( v (x) \), such that:

\[ \Sigma : D = \sigma : d (x) = \pi (d (v^*), \bar{x}) \] (2.18)

Then it can be shown (theorem of association, [86]) that:

\[ \forall x \in V, \quad \sigma (x) : d (x) = \sup_{\sigma \in \tilde{G}(x)} \sigma : d = \pi (d (x)) \] (2.19)

and

\[ \forall \Sigma^* \in \tilde{G}, \quad \Sigma^* : D \leq \Sigma : D \] (2.20)

Inequality (2.20) shows that any macroscopic stress \( \Sigma^* \in G \), which is both statically admissible and strength compatible in the sense of (2.6), is likely to underestimate the maximum dissipation capacity of the composite material at plastic collapse, defined by:

\[ \Pi^{\text{hom}} (D) = \sup_{\Sigma \in \tilde{G}} \Sigma : D \] (2.21)

and thus, making use of the duality of the strength and dissipation capacity definition of the strength domain:

\[ \tilde{G} = G^{\text{hom}} \] (2.22)

Relation (2.21) is the macroscopic counterpart of (2.9); and the solution of the yield design

---

\(^1\) More precisely, we consider the case where we can find \( \epsilon > 0 \) such that:

\[ \forall v^* \in \mathcal{K}, \quad \Sigma : D \leq (1 - \epsilon) \pi (d(v^*), \bar{x}) < \pi (d(v^*), \bar{x}) \]
problem thus reads:
\[ \Sigma : D = \Pi^{\text{hom}}(D); \quad \Sigma = \frac{\partial \Pi^{\text{hom}}}{\partial D} \] (2.23)

2.1.4 Limit Analysis

In contrast to the stress-strength approach, which provides a lower bound approach to the actual dissipation capacity (2.21), a kinematics approach to the plastic collapse provides an upper bound estimate of this maximum dissipation capacity. Such an approach is based on the normality rule of plastic flow. That is, at plastic collapse, the actual strain rate \( d \) (which derives from a kinematically admissible velocity field) is defined by a plastic flow rule that respects the normality rule:

\[ d \text{ def} = d^p = \hat{\lambda} \frac{\partial f}{\partial \sigma}(\sigma) \] (2.24)

where \( \hat{\lambda} \) is the plastic multiplier. Considering the normality rule is equivalent to considering that the material, at plastic collapse, exhausts its dissipation capacity at the highest (yet finite) rate. This is known as the principle of maximum plastic work. Furthermore, as a consequence of the convexity of \( f(\sigma) \), we have, for a given strain rate, \( d^* \):

\[ \forall \sigma \in G \quad \sigma : d^* \leq \sup_{\sigma' \in G} \sigma' : d^* = \pi \left( d^* = \hat{\lambda} \frac{\partial f}{\partial \sigma^*}(\sigma^*) \right) \] (2.25)

where \( \sigma^* \) is the stress associated with \( d^* \).

Now, let us consider the set of velocity fields:

\[ \mathcal{K}(D) = \left\{ \psi^*(x) | \overline{d(\psi^*)} = D \right\} \] (2.26)

We note \( \Sigma \) the macroscopic stress solution the yield design problem and \( \psi(x) \) the associated velocity field solution. Taking any velocity field \( \psi^*(x) \in \mathcal{K}(D) \), we obtain from equation (2.15):

\[ \forall \psi^* \in \mathcal{K}(D) \quad \delta W = \sigma : d(\psi^*) = \Sigma : D \leq \pi(d(\psi^*), \overline{x}) \] (2.27)

whereas in the case of the velocity field solution to the problem we have (2.18):

\[ \delta W = \sigma : d(\psi) = \Sigma : D = \pi(d(\psi), \overline{x}) = \Pi^{\text{hom}}(D) \] (2.28)
Thus, combining the two later equations, we obtain:

\[
\forall \mathbf{v}^* \in \mathcal{K}(\mathbf{D}) \quad \Pi_{\text{hom}}(\mathbf{D}) = \pi(\mathbf{d}(\mathbf{v}), \mathbf{x}) \leq \pi(\mathbf{d}(\mathbf{v}^*), \mathbf{x})
\]  

(2.29)

The previous inequality shows that any velocity field which is kinematically admissible and related by the normality rule to the plastic flow, provides an upper bound estimate of the actual dissipation capacity the RVE can afford at plastic collapse:

\[
\Pi_{\text{hom}}(\mathbf{D}) = \inf_{\mathbf{v}^* \in \mathcal{K}(\mathbf{D})} \pi(\mathbf{d}^* = \mathbf{d}(\mathbf{v}^*), \mathbf{x})
\]  

(2.30)

Finally, the derivation here is based on the homogeneous stress boundary condition (2.1), without any further restriction imposed on the velocity field than relation (2.8). For reasons to appear later on, it is useful to restrict the velocity fields to those that can be associated with a regular strain rate boundary condition, namely:

\[
\mathcal{K}(\mathbf{D}) = \{ \mathbf{v}^*(\mathbf{x}) \mid \mathbf{v}^*(\mathbf{x}) = \mathbf{D} \cdot \mathbf{x} \text{ on } \partial V \}
\]  

(2.31)

This restriction satisfies Eq. (2.8), and if considered as a boundary condition, it is known from the Hill Lemma that it does not affect the expression of the external work rate (2.7), which according to yield design theory is entirely dissipated into heat form at plastic collapse. But rather than a true velocity boundary condition (which contradicts the very nature of plastic collapse), the regular strain rate condition (2.31) imposed on the boundary of the RVE should be understood as a constraint to which the optimization problem (2.30) is subjected.
2.2 Variational Approach

2.2.1 Variational Formulation

The homogenization problem requires the solution of the following set of equations for an RVE composed of $i = 1, N$ material phases:

\begin{align*}
\nabla \cdot \sigma &= 0 \quad \text{in } V \tag{2.32a} \\
\sigma(x) &= \frac{\partial \pi_i}{\partial \mathbf{d}}(\mathbf{d}(\mathbf{z})) \quad \text{in } V_i \tag{2.32b} \\
\mathbf{d} &= \frac{1}{2}(\nabla \mathbf{v} + \nabla^T \mathbf{v}) \quad \text{in } V \tag{2.32c} \\
\mathbf{v} &= \mathbf{D} \cdot \mathbf{z} \quad \text{on } \partial V \tag{2.32d}
\end{align*}

Multiplying (2.32a) with $\mathbf{v}^*$ and integrating over the RVE, it turns out that the kinematic limit analysis problem (2.30) is indeed a variational problem; that is:

\begin{equation}
\Pi_{\text{hom}}(\mathbf{D}) = \inf \frac{1}{|V|} \int_V \pi(\mathbf{z}, \mathbf{d}(\mathbf{v}^*)) \, dV = \inf_{\mathbf{v}^* \in \mathcal{K}(\mathbf{D})} \frac{\pi(\mathbf{z}, \mathbf{d}(\mathbf{v}^*))}{\mathbf{v}^*} \tag{2.33}
\end{equation}

where $\mathcal{K}(\mathbf{D})$ is defined by (2.31). On first sight the problem may appear to be formally identical to a problem of linear elasticity (see Appendix A, Eq. (A.21), page 175), if one replaces the strain rate $\mathbf{d}$ by the strain $\mathbf{\varepsilon}$, and the dissipation function $\pi(\mathbf{d})$ by a strain energy function, say $\omega(\mathbf{\varepsilon})$. However, there is a fundamental difference, which is that the dissipation function $\pi(\mathbf{d}) = \sup(\sigma : \mathbf{d})$ is a homogeneous function of degree 1 (i.e., $\pi(\lambda \mathbf{d}) = \lambda \pi(\mathbf{d})$), while the strain energy function $\psi(\mathbf{\varepsilon})$ of linear elasticity is typically a quadratic function, $\omega(\mathbf{\varepsilon}) = \frac{1}{2} \mathbf{\varepsilon} : \mathbf{C} : \mathbf{\varepsilon}$. The nonlinearity, therefore, introduced by relation (2.32b) excludes the use of linear homogenization techniques of elasticity. On the other hand, like any other nonlinear relation, it is possible to linearize it in a region of interest and then resort to linear techniques. The nonlinear medium is then compared to a suitably chosen linear one, the linear comparison composite. This approach is pursued in what follows.
2.2.2 Linear Comparison Composite

The idea of using a linear comparison composite together with a variational formulation was first introduced by Castañeda in 1991 [80]. It formulates the determination of $\Pi_{\text{hom}}$ as the solution of an elasticity problem with an infinite number of phases (i.e. the stiffness tensor $C(x)$ constantly varies with $x$ and is not a piecewise constant function anymore). Then, all comes down to finding the equivalent linear composite defined by the stiffness $C(x)$.

Let $\omega_0$ be the strain rate energy density function of a linear heterogeneous comparison composite with non-uniform stiffness tensor $C_0(x)$:

$$\omega_0(x,d) = \frac{1}{2} d : C_0(x) : d$$  \hspace{1cm} (2.34)

Since $\pi(x,\lambda d) = \lambda \pi(x,d)$ and $\omega_0(x,\lambda d) = \lambda^2 \psi(x,d)$, the difference $\pi(x,d) - \psi(x,d)$ goes to $-\infty$ for infinitely large strain rates. Then, let:

$$\nu(x,C_0) = \sup_{d} \{ \pi(x,d) - \omega_0(x,d) \}$$  \hspace{1cm} (2.35)

It is readily recognized that:

$$\forall x,d,C_0 \quad \pi(x,d) \leq \omega_0(x,d) + \nu(x,C_0)$$  \hspace{1cm} (2.36)

Therefore, taking the minimum over $C_0$, we have:

$$\pi(x,d) \leq \inf_{C_0>0} \{ \omega_0(x,d) + \nu(x,C_0) \}$$  \hspace{1cm} (2.37)

It can be shown that relation (2.37) saturates into an equality provided some mathematical assumptions regarding dissipation function $\pi$. Then, replacing in (2.33) $\pi$ by the r.h.s expression of (2.37) allows us to restate the variational problem in the form:

$$\Pi_{\text{hom}}(D) = \inf_{x^* \in D} \inf_{C_0>0} \{ \omega_0(x,d(x^*)) + \nu(x,C_0) \}$$  \hspace{1cm} (2.38)
or equivalently, after interchanging the sequence of minimization:

\[
\Pi^{\text{hom}}(D) = \inf_{C_0 > 0} \{ \mathcal{W}_0(D) + \mathcal{V}(C_0) \}
\]  

(2.39)

with:

\[
\mathcal{W}_0(D) = \inf_{\mathbf{x}^* \in \mathcal{K}(D)} \omega_0(\mathbf{x}, \mathbf{d}(\mathbf{x}^*))
\]  

(2.40a)

\[
\mathcal{V}(C_0) = \nu(x, C_0)
\]  

(2.40b)

Relation (2.39) informs us that the macroscopic dissipation function is the sum of the strain rate energy of a well chosen heterogeneous linear composite \( \mathcal{W}_0(D) \), and a term \( \mathcal{V}(C_0) \) measuring the non-linearity of the original material. The original variational problem (2.33) is thus replaced by one which consists in finding the best possible comparison composite that delivers the best infimum in the sense of (2.39). However, since \( C_0(x) \) varies continuously within the RVE, its implementation is at least as difficult as the original problem. Yet, the advantage of the problem formulation (2.39) is that it allows the implementation of discrete forms of \( C_0(x) \rightarrow C_i = C_0(\mathbf{x}_i) \). This is shown next.

2.2.3 Approximation by \( N \)-Phase Composite

The second part in Castañeda’s work on Linear Comparison Composite consists in approximating the solution \( \Pi^{\text{hom}}(D) \) by an estimate \( \hat{\Pi}^{\text{hom}}(D) \) based on a piecewise constant form of the stiffness \( C_0(x) \). The question which arises is how to choose the behavior of the \( N \) phases of the comparison composite. This has been the topic in particular of subsequent papers published in 1996 and 2001 [81][83].

Consider a piecewise constant form of the strain rate energy \( \omega_0(\mathbf{x}, \mathbf{d}) \), that is:

\[
\omega_0(\mathbf{x}, \mathbf{d}) = \sum_i \chi(\mathbf{x}) \omega_i(\mathbf{d})
\]  

(2.41)

where \( \chi(\mathbf{x}) \) is the characteristic function of each phase; that is \( \chi(\mathbf{x}) = 1 \) if \( \mathbf{x} \in V_i \) and \( \chi(\mathbf{x}) = 0 \)
if $x \notin V_i$ (where $V_i$ is the domain occupied by phase $i$); while $\omega_i (d)$ is the strain rate energy of phase $i$:

$$\omega_i (d) = \frac{1}{2} d : C_i : d + \tau_i : d$$

(2.42)

with $C_i$ the stiffness of phase $i$ and $\tau_i$ a prestress, which will turn out useful for subsequent developments. From (2.39), it is understood that such a piecewise constant representation yields an upper bound of the actual dissipation capacity $\Pi(D)$. Indeed, recall that the infimum of two functions is always greater than or equal to the sum of the infimas of the two functions:

$$\inf_x (f(x) + g(x)) \geq \inf_x f(x) + \inf_x g(x)$$

(2.43)

Application of (2.43) to $\pi$ and $\psi - \pi$ yields:

$$\inf_{\mathbf{z}^* \in \mathcal{K}(D)} \omega_0 (x, d (\mathbf{z}^*)) \geq \inf_{\mathbf{z}^* \in \mathcal{K}(D)} \pi (x, d (\mathbf{z}^*)) + \inf_{\mathbf{z}^* \in \mathcal{K}(D)} \omega_0 (x, d (\mathbf{z}^*)) - \pi (x, d (\mathbf{z}^*))$$

(2.44)

where we recognize $\Pi^{\text{hom}}(D)$ and $\mathcal{W}_0(D)$; that is:

$$\Pi^{\text{hom}}(D) \leq \mathcal{W}_0(D) - \inf_{\mathbf{z}^* \in \mathcal{K}(D)} \omega_0 (x, d (\mathbf{z}^*)) - \pi (x, d (\mathbf{z}^*))$$

(2.45)

Now if we focus on the last term, we can overestimate it with:

$$- \inf_{\mathbf{z}^* \in \mathcal{K}(D)} \omega_0 (x, d (\mathbf{z}^*)) - \pi (x, d (\mathbf{z}^*)) \geq - \inf_{\mathbf{z}^* \in \mathcal{K}(D)} \omega_0 (x, d (\mathbf{z}^*)) - \pi (x, d (\mathbf{z}^*)) = \sup_{\mathbf{z}^*} \omega_0 (x, d (\mathbf{z}^*)) - \pi (x, d (\mathbf{z}^*))$$

(2.46)

$$= \sum_i \phi_i \mathcal{V}_i$$

where $\mathcal{V}_i$ is constant in each phase of volume fraction $\phi_i$:

$$\mathcal{V}_i = \sup_d \pi_i (d) - \omega_i (d)$$

(2.47)

Finally, for any comparison composite, we obtain the following upper bound for $\Pi^{\text{hom}}$:

$$\Pi^{\text{hom}}(D) \leq \mathcal{W}_0(D) + \sum_i \phi_i \mathcal{V}_i$$

(2.48)
Contrary to (2.39), expression (2.48) does not saturate into an equality. It is an upper bound for any comparison composite. The goal, therefore, is to find the comparison composite that will lead to the lowest possible upper bound, thus yielding the best possible estimate of $\Pi^{\text{hom}}$. However, as discussed by Castañeda [83], preserving a true upper bound status may sometimes turn out difficult, and we can replace the infima or maxima by just stationary points. The resulting estimates are then stationary variational estimates and not bounds in general. This new estimate, $\Pi^{\text{hom}}$, reads:

$$\Pi^{\text{hom}}(D) = \text{stat}_{\mathcal{C},\pi_i} \left[ W_0(D) + \sum_i \phi_i \mathcal{V}_i \right]$$

with

$$\mathcal{V}_i = \text{stat} \{ \pi_i(d) - \omega_i(d) \}$$

There are usually different points of stationary, which is why each particular case must be analyzed separately [83].

### 2.3 Effective Strain Rate Approach

#### 2.3.1 Secant Formulation

An alternative approach to approximating the actual dissipation capacity of the RVE, is to realize that the problem (2.32) is akin to a viscous flow problem, in which the solid’s behavior is described by a viscous constitutive law:

$$\sigma = \frac{\partial \pi(d)}{\partial d} = \mathcal{C}(d) : d$$

where $\mathcal{C}(d)$ is the forth order tensor of viscosity coefficients. Since $\pi(d)$ is a homogeneous function of degree 1 (i.e., Eq. (2.11)), this tensor obeys to:

$$\mathcal{C}(d) \sim \frac{1}{d}$$

For instance, if the dissipation function $\pi(d)$ depends on the first two invariants of the strain rate tensor, namely the volume strain rate $d_v = \text{tr} d = I^t_1$ and the norm of the deviator strain...
rate \( d_d = \sqrt{\delta \cdot \delta} = \sqrt{2J_2} \) (with \( \delta = d - d_v \)), such that \( \pi = \pi (d_v, d_d) \) we have:

\[
\sigma = \frac{\partial \pi}{\partial d_v} (d_v, d_d) \mathbf{1} + \frac{1}{d_d} \frac{\partial \pi}{\partial d_d} (d_v, d_d) \delta = \mathbb{C} (d) : \mathbf{d}
\]

(2.53)

where:

\[
\mathbb{C} (d) = 3\kappa (d_v, d_d) \mathbb{1} + 2\mu (d_v, d_d) \mathbb{K}; \quad \text{with}
\]

\[
\begin{cases}
\kappa (d_v, d_d) = \frac{1}{d_v} \frac{\partial \pi}{\partial d_v} (d_v, d_d) \\
\mu (d_v, d_d) = \frac{1}{2d_d} \frac{\partial \pi}{\partial d_d} (d_v, d_d)
\end{cases}
\]

(2.54)

This approach was pioneered by Suquet and is often called the Secant Method [95] [82], due to the nonlinear dependence of the stiffness-viscosity coefficients \( \kappa \sim 1/d_v \) and \( \mu \sim 1/d_d \) on \( d_v \) and \( d_d \), which for large strain rates, corresponding to the plastic collapse, tend to zero (see Eq. (2.52)). The approach has been extensively adopted by Dormieux and co-worker for the strength homogenization of porous materials [3] [88]. A closer look on the approach, however, reveals that it has much in common with Castañeda's comparison composite formulation.

### 2.3.2 Link with Comparison Composite Theory

Indeed, the approach can be seen as a particular case of Castañeda's comparison composite theory, in the sense that the stiffness \( \mathbb{C} (d) \) is evaluated at a reference strain rate, called the effective strain rate:

\[
\mathbb{C} (d (x)) \rightarrow \mathbb{C} (d^*)
\]

(2.55)

In other words, the determination of the stiffness \( \mathbb{C} (d (x)) \) of the best linear composite in Castañeda's approach, is here replaced by the determination of the optimal effective strain rate \( d^* \), assumed constant per phase. Yet, as shown by Suquet [95], the approach actually comes to evaluate the infimum and supremum in (2.45) and (2.47) at stationary points defined by the effective strain rate:

\[
\tilde{\Pi}^{\text{hom}} (D) = \text{stat} \tilde{C}_i \left( \mathcal{W}_0 (D) + \sum_i \phi_i \nu_i \right)
\]

(2.56)

where:

\[
\nu_i = \text{stat} \left\{ \pi_i (d) - \omega_i (d) \right\}
\]

(2.57)
In fact, the stationary conditions provide an optimality condition for the choice for the effective strain rate. Indeed, consider a linear comparison composite, that is, \( \omega_i(d) = \frac{1}{2} d : C_i : d = \frac{1}{2} \kappa_i d_v^2 + \mu_i d_d^2 \). Application of the stationary condition (2.57) comes to derive \( V_i \) w.r.t. its arguments:

\[
V_i = \text{stat} (\pi_i (d_v, d_d) - \psi_i (d_v, d_d)) \Rightarrow \begin{cases}
\frac{\partial \pi_i}{\partial d_v} - \kappa_i d_v = 0 \\
\frac{\partial \pi_i}{\partial d_d} - 2 \mu_i d_d = 0
\end{cases}
\] (2.58)

The stationary condition of \( V_i \), therefore, turns out to deliver the same relation as (2.54) employed in the secant formulation. In return, this implies that \( V_i \) at its stationary value reads:

\[
V_i = \pi_i (d'_v, d'_d) - \left( \frac{1}{2} \kappa_i (d'_v)^2 + \mu_i (d'_d)^2 \right)
\] (2.59)

Consider now the stationary condition (2.56):

\[
\Pi^\text{hom}(D) = \text{stat} \left( \frac{\partial \pi_0 (D)}{\partial \kappa_i} + \sum_i \phi_i \frac{\partial \psi_i (D)}{\partial \mu_i} \right) \Rightarrow \begin{cases}
\frac{\partial \pi_0 (D)}{\partial \kappa_i} + \phi_i \frac{\partial \psi_i (D)}{\partial \mu_i} = 0 \\
\frac{\partial \pi_0 (D)}{\partial \mu_i} + \phi_i \frac{\partial \psi_i (D)}{\partial \mu_i} = 0
\end{cases}
\] (2.60)

Let us note that,

\[
\frac{\partial \pi_0 (D)}{\partial \mu_i} = \frac{\partial}{\partial \mu_i} \sum_i \chi (x) \omega_i (d) = \phi_i \overline{d^V_d}
\] (2.61)

where \( \overline{d^V_d} = \frac{1}{V} \int_{V_i} d^2 dV \). Then, using (2.59) in (2.60) allows a closer inspection of the derivatives of \( V_i \); for instance

\[
\frac{\partial V_i}{\partial \mu_i} = - (d'_d)^2 + \frac{\partial d'_v}{\partial \mu_i} \left[ \frac{\partial \pi}{\partial d_v} (d'_v, d'_d) - \kappa_i d'_v \right] + \frac{\partial d'_d}{\partial \mu_i} \left[ \frac{\partial \pi}{\partial d_d} (d'_v, d'_d) - 2 \mu_i d'_d \right]
\] (2.62)

The two terms in parenthesis on the r.h.s are zero because of optimality condition (2.58). Finally, using (2.61) and (2.62) in the stationary condition (2.60) yields the following optimality
condition for the choice of an optimal deviatoric effective reference strain rate:

\[ \phi_i \bar{d}_d^{V_i} - \phi_i \left( d_d^r \right)^2 = 0 \]

\[ \downarrow \]

\[ \left( d_d^r \right)^2 = \bar{d}_d^{V_i} \]

An analogous relation can be derived for the volumetric effective reference strain rate:

\[ \left( d_v^r \right)^2 = \bar{d}_v^{V_i} \] (2.64)

In other words, the effective strain rates one should choose must be such that the corresponding linear comparison composite, subjected to homogeneous boundary conditions defined by \( D \), will have a second moment of its strain rate equal to the chosen effective strain rate. To illustrate this result, let us assume, for purpose of argument, that we use instead of the second moment, the mean of the strain rate of comparable magnitude. As depicted in Figure 2-2, the use of a linear comparison composite locally approximates the non-linear constitutive relation by a linear one. Now if we consider the strain rates taking place in the linear comparison composite subjected to the same boundary conditions as the non-linear material, and that we represent it with dots, these dots must lie in the region of good approximation of the non-linear constitutive relation. In case (a), the effective strain is suitably chosen whereas in case (b), the non-linearities are approximated in a certain region but the strain rates actually involved are in a different region. Equation (2.64), therefore, ensures that the approximation is accurate.

### 2.3.3 The Case of a Prestress

To close this Section on the effective strain rate approach, it is useful to remark that the consideration of a prestress in the expression of \( \omega_i (d) \) of the comparison composite, i.e. \( \omega_i (d) = \frac{1}{2} \kappa_i d_v^2 + \mu_i d_d^2 + \tau_i d_u \), slightly modifies the stationary conditions. In fact, instead of (2.58) and
Figure 2-2: Interpretation of the Effective Strain Rate Approach: Relations (2.63) and (2.64) ensure the accuracy of the approximation (case a).

(2.59), we would have obtained:

\[
\frac{\partial \pi_i}{\partial \epsilon_v} - \kappa_i \epsilon_v - \tau_i = 0
\]

\[
\downarrow
\]

\[
V_i = \pi_i (\epsilon_v, \epsilon_v) - \left( \frac{1}{2} \kappa_i (\epsilon_v)^2 + \mu_i (\epsilon_v')^2 + \tau_i \epsilon_v \right)
\]

The stationary condition (2.60) remains a priori unchanged, since:

\[
\frac{\partial W_0(D)}{\partial \kappa_i} + \phi_i \frac{\partial V_i}{\partial \kappa_i} = 0; \quad \text{with} \quad \left\{ \begin{array}{l}
\frac{\partial W_0(D)}{\partial \kappa_i} = \frac{1}{2} \phi_i \epsilon_v \epsilon_v' \\
\frac{\partial V_i}{\partial \kappa_i} = \frac{1}{2} (\epsilon_v')^2
\end{array} \right.
\]

(2.66)

However, as specified in (2.49), the stationary must also be achieved w.r.t. \( \tau_i \), that is:

\[
\frac{\partial W_0(D)}{\partial \tau_i} + \phi_i \frac{\partial V_i}{\partial \tau_i} = 0; \quad \text{with} \quad \left\{ \begin{array}{l}
\frac{\partial W_0(D)}{\partial \tau_i} = \phi_i \epsilon_v \\
\frac{\partial V_i}{\partial \tau_i} = -\epsilon_v'
\end{array} \right.
\]

(2.67)
We, thus, end up with two optimality conditions for the choice of the volumetric effective reference strain rate:

\[
(d'_v)^2 = \frac{d'^2 V_i}{d_v} \quad ; \quad d'_v = \frac{d V_i}{d_v}
\]  \hspace{1cm} (2.68)

To simultaneously satisfy both optimality conditions, \(d_v\) should be a constant field in phase \(V_i\). We should, however, keep in mind that the stationary condition may be a non optimal local minimum, and not an infimum in the sense of yield design theory. Furthermore, the presented derivation of the optimality conditions for the choice of an effective reference strain rate is based on some restrictive assumptions: (i) the expressions of the stiffness coefficients are possible (\(\kappa\) and \(\mu\) positive), and (ii) \(\kappa\) and \(\mu\) are independent of each other (allowing an independent differentiation). As we will show in the next Chapter, this is not always the case; which is why we will not use the effective strain rate approach, but the less restrictive Linear Comparison Composite Theory.

### 2.4 Chapter Summary

From this review of the elements of strength homogenization it appears to us that the variational formulation of Castañeda based on the Linear Comparison Composites is most suitable for our purpose, which is the strength homogenization of strength properties of multiscale heterogeneous materials. The key to the determination of the macroscopic strength domain is the stationary condition (2.49), which provides an appropriate estimate of the plastic dissipation potential of the composite material:

\[
\bar{\Pi}^{\text{hom}}(D) = \text{stat} \min \bigg[ \mathcal{W}_0(D) + \sum_i \phi_i V_i \bigg]
\]  \hspace{1cm} (2.69)

The determination of \(\bar{\Pi}^{\text{hom}}(D)\) requires as input two quantities:

1. The expression of the macroscopic strain rate energy \(\mathcal{W}_0(D)\), which needs to be determined for each particular representation of a heterogeneous material from its (linear) definition (2.40a), (2.41) and (2.42):

\[
\mathcal{W}_0(D) = \inf_{y^r \in \mathcal{K}(D)} \sum_i \phi_i \frac{1}{2} d : C_i : d + \tau_i : d
\]  \hspace{1cm} (2.70)
Given the linearity, we will make use here of the classical results of linear homogenization theory (see Appendix A), to link the microscopic strain rate \( \mathbf{d} \) by means of a linear operator to the macroscopic strain rate \( \mathbf{D} \):

\[
d(\mathbf{x}) = A(\mathbf{x}) : \mathbf{D}
\]

where \( A(\mathbf{x}) \) is the forth-order strain (rate) concentration tensor, which carries all relevant information about the morphology of the composite. This leads to explicit expressions of the strain rate energy \( W_0(\mathbf{D}) \).

2. The expression of the \( V_i \) function (constant per phase) as defined by (2.50), which has two components: the dissipation function \( \pi_i(\mathbf{d}) \), which depends on the strength domain of the phase, and the elastic expression (2.42) of \( \omega_i(\mathbf{d}) \); that is:

\[
V_i = \text{stat} \left\{ \pi_i(\mathbf{d}) - \left( \frac{1}{2} \mathbf{d} : \mathbf{C}_i : \mathbf{d} + \tau_i : \mathbf{d} \right) \right\}
\]

Based on the so obtained expression of \( \Pi^\text{hom}(\mathbf{D}) \), the macroscopic stress yield stress \( \Sigma \) is obtained by differentiation, i.e. Eq. (2.23). A priori, this yield stress is not linked to the stress average in the comparison composite. However, because of stationary condition (2.49), we have, similarly to (2.62):}

\[
\Sigma = \frac{\partial \Pi^\text{hom}}{\partial \mathbf{D}}(\mathbf{D}) = \frac{\partial W_0}{\partial \mathbf{D}}(\mathbf{D})
\]

This shows that the macroscopic stress, in the comparison composite subjected to the macroscopic strain rate \( \mathbf{D} \), is equal to the actual yield stress.

Therefore, once the optimality conditions (2.49) is derived, we can use the constitutive behavior of the comparison composite in order to replace all the occurrences of \( \mathbf{D} \) by expressions involving the macroscopic yield stress \( \Sigma \). Then, this system of optimality conditions should

\[\text{2 The stationary estimate of } \Pi^\text{hom}, \text{ (2.49), depends on } \mathbf{D}, \kappa_i, \mu_i \text{ and } \tau_i \text{, such that:}
\]

\[
\frac{\partial \Pi^\text{hom}}{\partial \mathbf{D}} = \frac{\partial W_0}{\partial \mathbf{D}} + \frac{\partial \kappa_i}{\partial \mathbf{D}} \frac{\partial \mu_i}{\partial \kappa_i} \left[ W_0 + \sum_i \phi_i V_i \right] + \frac{\partial \mu_i}{\partial \mathbf{D}} \frac{\partial \tau_i}{\partial \mu_i} \left[ W_0 + \sum_i \phi_i V_i \right] + \frac{\partial \tau_i}{\partial \mathbf{D}} \frac{\partial \tau_i}{\partial \tau_i} \left[ W_0 + \sum_i \phi_i V_i \right]
\]

\[\text{in which the partial derivatives with respect to } \kappa_i, \mu_i \text{ and } \tau_i \text{ are zero, due to stationarity.} \]
Steps of Chosen Strength Homogenization Approach

1. Compute the macroscopic strain rate energy of the linear comparison composite, \( W_0(D) \), as a function of the stiffness parameters \( \kappa_i, \mu_i \).

2. Compute the expression of functions \( \pi_i \) and \( \mathcal{V}_i \) as a function of \( \kappa_i, \mu_i \).

3. Generate the system of equations from the stationary condition (2.49):

\[
\forall i = 1, N : \frac{\partial \Pi_{\text{hom}}}{\partial \kappa_i} = 0; \frac{\partial \Pi_{\text{hom}}}{\partial \mu_i} = 0; \frac{\partial \Pi_{\text{hom}}}{\partial r_i} = 0
\]

4. Replace each occurrence of \( D_e \) and \( D_d \) by their expressions in terms of \( \Sigma_m, \Sigma_d, \kappa_i, \mu_i \).

5. Solve the corresponding system of equation and obtain the macroscopic strength criterion.

Table 2.2: Summary: Strength homogenization procedure based on the Comparison Composite Theory

allow us to determine the best stiffness parameters for the comparison composite. We get as many equations as unknowns. Now, if this system of equations was consistent, we would obtain a given value for each stiffness parameter and therefore a given estimate for \( \Pi_{\text{hom}}(D) \) as a function of \( \Sigma \) (since we expressed all the equations as a function of \( \Sigma \)). And since the same \( \Sigma \) is associated with any strain rate of the form \( \lambda D \), we get the same estimation of \( \Pi_{\text{hom}}(\lambda D) \) for any \( \lambda \). This would be in contradiction with the fact that \( \Pi_{\text{hom}} \) is a homogeneous function of degree 1. In fact, the system of equation is ill-conditioned (due to the homogeneity of each microscopic dissipation function) and instead of giving us a value for each stiffness parameter it gives us \( N - 1 \) relations between the \( N \) comparison stiffness parameters and 1 relation between the different invariants of \( \Sigma \), which is the sought macroscopic strength criterion.

Table 2.2 summarizes the main steps of the procedure for the isotropic case, which will be put to work in the next Chapter for the multiscale homogenization of strength properties of shale.
Chapter 3

Multiscale Strength Homogenization of Shale

This second chapter on strength homogenization deals with the application of strength homogenization theory to shale. Shale, the sealing formation in most hydrocarbon reservoirs, is a highly heterogeneous natural composite, with heterogeneities that manifest themselves from the nanosized porosity scale in between highly compacted clay particles to the microscale of silt-quartz inclusions. For the development of a homogenization model for strength, we reduce this complexity to a two-scale micromechanics model to which we apply in a step-by-step fashion the strength homogenization procedure outlined in the previous chapter (see Table 2.2). In particular, at the scale of the porous clay composite of shale (Level 'I'), we derive the strength domain of a composite composed of a cohesive-frictional solid and pores, which as we will see includes the elliptical and hyperbolic case. Then, in a second homogenization step (Level 'II'), we homogenize the strength behavior of the porous clay and rigid inclusions (with and without adhesion) to obtain an estimate of shale macroscopic strength behavior.

3.1 Multiscale Thought Model for Shale

Shale is a multi-phase, multi-scale, transversely isotropic, and compositionally diverse sedimentary rock. It is composed primarily of sedimented clay particles, and some quantities of larger, silt-sized inclusions. The widely documented diversity of shale materials currently demands
detailed localized testing in engineering applications, motivating the need for improved understanding and predictive models. The aim of this chapter is to contribute a two-scale engineering micromechanics model for strength behavior of shale. The challenge of modeling the strength behavior of shale is to find the best description of the material, involving the least parameters. The model will have to capture the main factors governing the behavior of shales.

Figure 3-1 displays a three-level 'thought model' of the multiscale structure of shale materials [100], which will be the backbone of our model approach. This thought model spans roughly seven orders of magnitude, from the scale of the elementary particle (Level '0') to the scale of the macroscopic clay–silt inclusion composite (Level 'II'). The different scales satisfy the scale separability condition; that is:

$$J = I, II : L^{J-I} \ll L^J \ll L^{J+1}$$

(3.1)

where $L^J$ stands for the characteristic length scale of each level. In some more detail:

- Level '0' is the scale of elementary clay particles, and has classically been designated as the fundamental scale of clay mineralogy (see e.g. [48],[71]). While the structures of the clay minerals (kaolinite, illite, smectite, etc.) are reasonably well known, their mechanical properties are rarely documented in handbooks [68]. The small nature of clay particles in pure solid form becomes the main obstacle for performing direct measurements of mechanical properties of clay minerals.

- Level 'I' is the scale of the porous clay composite which manifests itself at the sub-micrometer scale. This scale is classically the scale of advanced observational methods, e.g. scanning electron microscopy (SEM) and transmission electron microscopy (TEM), which aim at linking the morphology of the clay fabric to physicochemical, electrochemical, bio-organic, and burial diagenesis processes [8],[71]. SEM images reveal the varying configurations of the porous clay composite, ranging from highly ordered sheet bundles to wavy flake structures, with characteristic dimensions of clay sheets of 500–1000 nm and 20–50 nm thick [100]. The corresponding aspect ratio of clay particles is approximately $1/25 - 1/20$. Through mercury intrusion porosimetry (MIP) testing, it has been determined that the space in between clay sheets accounts for almost the totality of the
Figure 3-1: Multiscale structure thought model of shale (adapted from [77])
porosity in shale, with characteristic pore access radii of some nanometers [50]. The volume fraction of the solid clay is denoted by $\eta$, and the volume fraction of voids by $\varphi = 1 - \eta$.

- Level ‘II’ is the macroscopic scale of characteristic size in the sub-millimeter and millimeter range. At this scale, the material is composed of the porous clay fabric intermixed with an abundant population of poorly sorted detrital grains (quartz inclusions), which are either concentrated into laminations located between thinner, clay-rich lens shaped lams or homogeneously distributed throughout. We denote by $f_{inc}$ the silt volume fraction. As quartz and silt are much stiffer and much stronger than the porous clay phase, it is reasonable to consider, for the purpose of strength homogenization, these inclusions as rigid. In return, the behavior of the interface between the inclusions and the porous clay phase may affect the macroscopic strength behavior. For this reason, two extreme conditions will be considered in the strength homogenization approach: perfect adherence and slippery imperfect interface.

It is readily recognized that the success of predicting shale strength behavior relies on bridging these different scales. This will be achieved through a two-scale homogenization approach, Level I–homogenization and Level II–homogenization, based on the scale separability condition (3.1).

### 3.2 Level ‘0’: Pressure Sensitive Strength Behavior

There is little known about the strength behavior of single clay crystals; but it is generally agreed, in the geomechanics community, that clay is a pressure sensitive material, meaning that the shear strength increases with increasing confining pressure. Pressure sensitivity is classically captured, in strength of materials, through the concept of friction (see Table 3.1).

#### 3.2.1 Bulk Frictional Behavior: Mohr-Coulomb and Drucker-Prager Criterion

Two famous strength criteria translate a bulk frictional behavior into stress space: the Mohr-Coulomb criterion and the Drucker-Prager criterion. Both carry the idea that the maximum
Friction

The concept of friction was first studied by Leonardo Da Vinci (1452-1519). He stated the two basic laws of friction: (i) the area of contact has no effect on friction; (ii) if the load of an object is doubled, its friction will also be doubled. Guillaume Amontons (1663-1705) also came up with an original set of theories. He believed that friction was predominately a result of the work done to lift one surface over the roughness of the other, or from the deforming or the wearing of the other surface. The work of Charles August Coulomb (1736-1806) completed the one of Amontons leading to the "Amontons-Coulomb Law" for the contact between two solids:

\[ F = \mu N \]

where the frictional force, \( F \), is proportional to the normal force, \( N \), but independent of the area of the sliding bodies. \( \mu \) is commonly known as the coefficient of friction. F. Philip Bowden and David Tabor (1950) gave a physical explanation for the laws of friction. They determined that the true area of contact is a very small percentage of the apparent contact area. The true contact area is formed by asperities. As the normal force increases, more asperities come into contact and the average area of each asperity contact grows. The frictional force was found to be dependent on the true contact area, a much more intuitively satisfying argument than what the Amontons-Coulomb law allows. Bowden and Tabor argued that within these asperities all of the dynamics of friction takes place.

While much progress has been made in recent years, namely through the invention of the Atomic Force Microscopy in 1986, enabling scientists to study friction at atomic scale, the actual origin of friction is still a subject of active research.

Table 3.1: Background: Friction (adapted from [113])
shear a material can support depends on the confining pressure. The Mohr-Coulomb criterion is a surface stress criterion reading:

\[ f(T = \sigma \cdot n) = |T_t| + \mu T_n - C \leq 0 \quad (3.2) \]

where \( T_t = t \cdot (\sigma \cdot n) \) is the tangential shear stress on the material surface oriented by unit outward normal \( n \), \( T_n = n \cdot (\sigma \cdot n) \) is the normal stress acting on this surface, \( \mu = \tan \varphi \) is the Mohr-Coulomb friction coefficient, and \( \varphi \) is the Mohr-Coulomb friction angle. Another way of writing the Mohr-Coulomb criterion is in form of the principal stresses, \( \sigma_I \geq \sigma_{II} \geq \sigma_{III} \):

\[ f(\sigma) = \sigma_I - \sigma_{III} + (\sigma_I + \sigma_{III}) \sin \varphi - 2C \cos \varphi \leq 0 \quad (3.3) \]

The Drucker-Prager criterion can be viewed as a Mohr-Coulomb criterion on the deviatoric stress plane oriented by the orientation of the hydrostatic axis, i.e. \( n = \frac{1}{\sqrt{3}} (u_I + u_{II} + u_{III}) \), with \( u_I \) the eigenvectors of the stress tensor corresponding to principal stress directions. In contrast to the Mohr-Coulomb criterion, the confining stress on the deviator stress plane is the mean stress, \( \sigma_m = \frac{1}{3} I_1 = \frac{1}{3} \text{tr}(\sigma) = \frac{1}{3} (\sigma_I + \sigma_{II} + \sigma_{III}) \), involving thus the three principal stresses. The shear stress magnitude on the deviator plane is expressed by the norm \( \sigma_d = \sqrt{s : s = \sqrt{\text{tr}(s \cdot s)} \) of the stress deviator, \( s = \sigma - \sigma_m 1 \), respectively by the second invariant of \( s, J_2 = \sigma_d^2/2 \); so that:

\[ f(\sigma) = \sqrt{J_2} + \alpha \sigma_m - c \leq 0 \quad (3.4) \]

\( \alpha \) is called the friction coefficient, and \( c \) is the cohesion. It is important to note that there is a limitation on the choice of the friction coefficient,

\[ \alpha < \sqrt{\frac{3}{4}} \quad (3.5) \]

Indeed, it has been shown that this value corresponds to a friction angle of \( \varphi = 90^\circ \) for the corresponding Mohr-Coulomb criterion [34]. Interestingly, the expression \((3 - 4\alpha^2)\) spontaneously comes very often out in subsequent derivations; and it is useful to keep in mind that this term needs to be always positive.

Furthermore, it will turn out useful to link the Drucker-Prager friction coefficient \( \alpha \) to the
Mohr–Coulomb friction coefficient $\tan \phi$, by considering the deviator plane representation of both criteria (3.3) and (3.4), as shown in Figure 3-2. Considering respectively the internal cone and the compression cone of the Drucker-Prager criterion, yields the following links between the material properties of the Drucker-Prager material $(c, \alpha)$ and of the Mohr-Coulomb criterion $(C, \sin \varphi)$ [90]:

\[
\begin{align*}
\text{Compression Cone} & : C &= \frac{3 - \sin \varphi}{2\sqrt{3} \cos \varphi} \quad \sin \varphi = \frac{3\alpha}{\alpha + 2\sqrt{3}} \\
\text{Internal Cone} & : C &= \sqrt{\frac{3 + (\sin \varphi)^2}{3 (\cos \varphi)^2}} \quad \sin \varphi = \sqrt{\frac{3\alpha^2}{3 - \alpha^2}}
\end{align*}
\]

Finally, from a practical point of view, the Drucker-Prager model involves only regular functions of the principal stresses, and it is usually easier to handle than the Mohr-Coulomb criterion. From a more fundamental perspective, recent results of micromechanics show that the continuum Drucker-Prager criterion may well represent an averaged form of a Mohr-Coulomb interface criterion between rigid particles organized in a polycrystal way [41],[66],[67]. This
result is briefly evoked here below.

### 3.2.2 Micromechanics Foundation

The choice of modeling the clay particles as a homogeneous phase following a Drucker-Prager criterion may find a theoretical foundation in the work of Fritsch et al. [41] and Maalej [66].

Fritsch et al. studied the brittle failure of a polycrystal material with weak interfaces (Fig. 3-3(a)). The crystals themselves are assumed to behave linear elastic, and the interfaces as well, so that the interface traction $T(x) = \sigma \cdot n$ is related to the displacement discontinuity $[[\xi]](x)$ by:
where $K$ is the interface stiffness tensor:

$$K = K_{n_1} \otimes \mathbf{n}_1 + K_t (1 - \mathbf{n}_1 \otimes \mathbf{n}_1), \quad K_n \to \infty$$

(3.8)

The interface is assumed to fail in a brittle manner once the shear stress $T_{i} = t \cdot (\sigma \cdot n)$ at this interface reaches a threshold defined by a criterion of the Mohr-Coulomb type (3.2):

$$\forall \mathbf{x} \in \mathcal{I}, \quad T_{i} (\mathbf{x}) \leq T_{i}^\sigma = C - \mu \Sigma_n (\mathbf{x})$$

(3.9)

Application of the polycrystal model with weak interfaces to the problem yields a Drucker-Prager type criterion for the onset of brittle failure of the polycrystal-interface composite, which involves the second invariant of the macroscopic stress deviator $\sqrt{J_2} = \frac{1}{2} \Sigma : \Sigma$ (with $\Sigma = \Sigma - \Sigma_m \mathbf{1}$) and the macroscopic mean stress $\Sigma_m = \frac{1}{2} I_1 = \frac{1}{3} \text{tr} \Sigma$:

$$B_{T_i} \sqrt{J_2} \leq C - \mu \Sigma_m$$

(3.10)

where $B_{T_i}$ is a concentration factor which depends on the interfacial rigidity, $\kappa$, and the crystal compressibility, $\chi$, and which varies between 0 and $\sqrt{\frac{2}{5}}$ (Fig. 3-3(b)).

A similar result was obtained by Maalej [66], by application of the effective strain rate approach of strength homogenization (see Section 2.3) to a polycrystal porous materials with interfaces whose behavior is governed, in compression, by the Amontons-Coulomb law for non cohesive frictional interfaces (see Table 3.1):

$$|T_{i}| \to -\mu T_n$$

(3.11)

In contrast to the brittle failure approach of Fritsch et al. [41], this approach is associated with a ductile failure of the interfaces in the sense of yield design theory. The result, however, is quite the same, namely a Drucker-Prager type criterion without cohesion for the composite behavior of the porous polycrystal with interfaces:
\sqrt{J_2} + T \sigma_m \leq 0 \quad (3.12)

where \( T = T (\mu, \eta) \) is recognized as a macroscopic friction coefficient in the sense of the Drucker-Prager model.\(^1\)

These recent results of advanced micromechanics show that a Drucker-Prager criterion can be seen as a representation of a distinct weakness of the intercrystalline interfaces at smaller scales. It is in this sense that we employ, in what follows, the Drucker-Prager strength model to describe the strength domain of the polycrystal clay particles at level '0'. The dual definition of the strength domain is given by:

\[
\sigma \in G_s (x) \Leftrightarrow \begin{cases} 
    f (\sigma) = \sqrt{J_2} + \alpha_s \sigma_m - c_s \leq 0 \\
    \pi (d) = \sup (\sigma : d) = \begin{cases} 
        \frac{c_s}{\alpha_s} d_v & \text{if } d_v \geq \sqrt{2} \alpha d_d \\
        \infty & \text{else}
    \end{cases}
\end{cases} \quad (3.13)
\]

where subscript \( s \) stands for ‘solid’, \( \alpha_s < \sqrt{3}/2 \) is the solid’s friction coefficient, \( c_s \) is the solid’s cohesion, \( J_2 = \frac{1}{2} \text{tr} (s \cdot s) \) and \( \sigma_m = \frac{1}{3} I_1 = \frac{1}{3} \text{tr} (\sigma) \) are stress invariants of the micro-stress tensor \( \sigma = s + \sigma_m \mathbf{1} \), while \( d_d = \sqrt{\delta : \delta} = \sqrt{2J_2} \) and \( d_v = \text{tr} (d) \) are the strain rate invariants of the micro-strain rate tensor \( d = \delta + \frac{1}{3} d_v \mathbf{1} \).

### 3.3 Level I – Homogenization

The focus of this section is the Level I strength homogenization of a porous material composed of a solid phase that follows the Drucker-Prager strength model and voids. The problem is a prominent problem in the strength homogenization literature, starting with Gurson’s hollow sphere model for a Von-Mises solid phase \([49][61]\) (see also \([47][99]\)). Most recent contributions

\(^1\)The expression derived by Manlej reads:

\[
T = \sqrt{\frac{3 \mu^2}{2 \eta^2 (2 - 3 \eta)} - \frac{3 (1 - \eta)}{4 \eta}}
\]

where \( \eta \) is the granular packing density. It is readily found that function \( T \) is singular at \( \eta = 2/3 \), and that it yields a negative value for the macroscopic friction coefficient for higher packing densities \( \eta > 2/3 \).
that consider the Drucker-Prager criterion are due to Dormieux and co-workers [3], [38], employing the effective strain rate approach of strength homogenization (see Section 2.3). This Section takes a 'new' look on this 'old' problem — using the Linear Comparison Composite approach outlined in Chapter 2.

3.3.1 Hyperbolic Regularization of the Drucker-Prager Criterion and \( \pi \) Function

A necessary condition for the application of the variational approach to strength homogenization is that the strength domain is strictly convex. This is not the case of the Drucker-Prager strength criterion (3.13), and in addition the function has a point of singularity at \( (J_2 = 0; I_1 = \frac{3 \alpha_s}{\alpha_s}) \). A convenient way to circumvent this drawback is to introduce a family of regular strength criteria that asymptotically tend to the Drucker-Prager criterion. This is here achieved by considering a family of hyperbolas, as shown in Figure 3-4, of the form:

\[
f(\sigma) = 1 - \left( \frac{\sigma_m - S_0}{A} \right)^2 + \left( \frac{\sigma_d}{\sqrt{2B}} \right)^2 \leq 0
\]  

(3.14)

where \( \sigma_d = \sqrt{2J_2} \). The Drucker-Prager criterion is obtained by letting:

\[
\begin{cases}
B = \alpha_s A \\
S_0 = \frac{c_s}{\alpha_s} \\
A \to 0
\end{cases}
\]

(3.15)

We now seek for the corresponding dual definition of the strength domain, in terms of the \( \pi \) function, from the following set of equations:

\[
d = \lambda \frac{\partial f}{\partial \sigma}(\sigma)
\]  

(3.16a)

\[
f(\sigma) = 0
\]  

(3.16b)

\[
\sigma : d = \pi(d)
\]  

(3.16c)

The \( 6 + 1 + 1 = 8 \) equations allow solving for the 8 unknowns: \( \pi(d), \lambda \) and \( 6 \times \sigma_{ij} \) at the
Figure 3-4: Approximation of a Drucker-Prager strength domain by a family of hyperbolic strength domains.

boundary of the strength domain. In particular, in the case of the hyperbolic strength criterion (3.14), we make use of the fact that:

$$\frac{\partial f}{\partial \sigma} (\sigma) = \frac{1}{3} \frac{\partial f}{\partial \sigma_m} (\sigma_m, \sigma_d) \left(1 + \frac{\partial f}{\partial \sigma_d} (\sigma_m, \sigma_d) \frac{s}{\sigma_d}\right)$$

(3.17)

Thus, Eq. (3.16a) gives:

$$\begin{cases}
\sigma_m - S_0 = \frac{A^2}{\lambda} d_{\sigma} \\
s = \frac{B^{2\lambda}}{\delta \lambda}
\end{cases}$$

(3.18)

While the value of $\delta$ is given by Eq (3.16b):  

$$\left(\frac{\sigma_m}{\delta}\right)^2 = \left(\frac{A d_v}{2}\right)^2 - \left(\frac{B d_d}{\sqrt{2}}\right)^2$$

(3.19)
It follows:

\[
\pi_s(d) = \pi(d_v, d_d) = S_0d_v - \sqrt{(Ad_v)^2 - (\sqrt{2Bd_d})^2}
\]  

(3.20)

with \( d_v = \text{tr} \, d = I_1^t \) and \( d_d = \sqrt{\delta : \delta} = \sqrt{2J_2^t} \). Without difficulty we verify that (3.20) reduces to \( \pi(d) = (c_s/\alpha_s) \, d_v \) for the Drucker-Prager conditions (3.15); which is the \( \pi - \) function expression (3.13).

Expressions (3.14) and (3.20) will turn out useful not only for the Level I – homogenization, but for the Level II – homogenization as well.

### 3.3.2 Step 1: Strain Rate Energy Function \( \mathcal{W}_0(D) \) of the Porous Clay Composite

This and the next sections show in a step-to-step fashion the application of the chosen strength homogenization procedure summarized in Table 2.2. The first step consists in determining the strain rate energy function \( \mathcal{W}_0(D) \) of the linear comparison composite (LCC), subjected to a regular strain rate boundary condition (2.32d):

\[
\forall x \in \partial V : \mathbf{u}(x) = D \cdot \mathbf{x}
\]  

(3.21)

Consider the porous clay composite composed of a solid phase (volume fraction \( \eta \)) and porosity \( \varphi = 1 - \eta \). It is convenient to apply a continuous description of the microscopic stresses:

\[
\sigma(x) = \mathbf{C}(x) : \mathbf{d}(x) + \tau(x)
\]  

(3.22)

where \( \mathbf{C}(x) \) and \( \tau(x) \) are respectively the stiffness and the eigenstress whose spatial distribution within the RVE is given by:

\[
\mathbf{C}(x) = \begin{cases} C_s = 3\kappa I + 2\mu K & (V_s) \\ 0 & (V_p) \end{cases} \quad \tau(x) = \begin{cases} \tau_1 & (V_s) \\ 0 & (V_p) \end{cases}
\]  

(3.23)

where \( V_s \) and \( V_p \) stand respectively for the domain occupied by the solid phase and the voids.

Using classical results of linear micromechanics, the corresponding macroscopic stress equa-
tion of state reads:

$$\Sigma = C^{\text{hom},I} : D + T^I$$  \hspace{1cm} (3.24)

where $C^{\text{hom},I}$ and $T^I$ are respectively the macroscopic stiffness tensor and the macroscopic prestress given by:

$$C^{\text{hom},I} = \overline{C}(\bar{x}) : \overline{A}(\bar{x}) = C_s : \eta \overline{A}^s = 3\kappa^I J + 2\mu^I K$$  \hspace{1cm} (3.25a)

$$T^I = \overline{\tau}(\bar{x}) : \overline{A}(\bar{x}) = \tau 1 : \eta \overline{A}^s = \tau 1 : C_s^{-1} : C^{\text{hom},I} = \frac{\kappa^I}{\kappa} 1$$  \hspace{1cm} (3.25b)

with:

$$\kappa^I = \eta \kappa \overline{J} : \overline{A}^s$$ \hspace{1cm} (3.26a)

$$\mu^I = \eta \mu \overline{K} : \overline{A}^s$$ \hspace{1cm} (3.26b)

where $A(\bar{x})$ is the forth-order strain (rate) localization tensor and $\overline{A}^s$ the volume average of it over the solid phase. Let us note that a dimensional analysis of the homogenized stiffness properties (3.26) readily yields:

$$\kappa^I = \mu K_I \left( \frac{\kappa}{\mu} \eta \right)$$ \hspace{1cm} (3.27a)

$$\mu^I = \mu M_I \left( \frac{\kappa}{\mu} \eta \right)$$ \hspace{1cm} (3.27b)

where $\kappa/\mu$ is the bulk-to-shear modulus ratio of the solid phase, while the dimensionless functions $K_I$ and $M_I$ are Level I pore morphology factors, that depend on the bulk-to-shear modulus ratio, the pore morphology and the solid concentration $\eta$.

The strain rate energy function $W_0(D)$ is obtained in an analogous fashion from linear homogenization theory, starting with (2.70), which yields for the solid–void composite (see Appendix A, relation (A.130)):

$$W_0(D_v, D_d) = \frac{1}{2} \kappa^I D_v^2 + \mu^I D_d^2 + \frac{\kappa^I}{\kappa} \tau D_v + \frac{1}{2\kappa} \left( \frac{\kappa}{\kappa} - \eta \right) \tau^2$$  \hspace{1cm} (3.28)

$$= \frac{1}{2} \mu K_I D_v^2 + \mu M_I D_d^2 + \frac{\mu}{\kappa} K_I \tau D_v + \frac{1}{2\kappa} \left( \frac{\mu}{\kappa} K_I - \eta \right) \tau^2$$
where \( D_v = \text{tr}(D) \) and \( D_d = \sqrt{\Delta : \Delta} \) with \( \Delta = D - \frac{1}{3} D_v 1 \).

### 3.3.3 Step 2: \( \mathcal{V} \) Function for an Hyperbolic Criterion

The second step consists in determining the \( \mathcal{V} \) function (Eq. (2.50)) for the solid phase (\( \mathcal{V} \) for the pore space is zero):

\[
\mathcal{V}_s = \text{stat} \{ \pi_s(d) - \omega_s(d) \} \quad (3.29)
\]

What we need is (3.20) and a suitable expression for the strain rate energy of the solid:

\[
\omega_s(d) = \frac{1}{2} \kappa d_v^2 + \mu d_d^2 + \tau d_v \quad (3.30)
\]

Then, applying the stationary condition of the \( \mathcal{V} \) function yields:

\[
\frac{\partial \mathcal{V}}{\partial d_v} = \frac{\partial (\pi_s - \omega_s)}{\partial d_v} = S_0 - \frac{A^2 d_v}{\sqrt{(A_d v)^2 - (\sqrt{2} B d_d)^2}} - \kappa d_v - \tau = 0 \quad (3.31a)
\]

\[
\frac{\partial \mathcal{V}}{\partial d_d} = \frac{\partial (\pi_s - \omega_s)}{\partial d_d} = \frac{2 B^2 d_d}{\sqrt{(A_d v)^2 - (\sqrt{2} B d_d)^2}} - 2 \mu d_d = 0 \quad (3.31b)
\]

which implies:

\[
\kappa d_v + \tau = S_0 - \frac{A^2 d_v}{\sqrt{(A_d v)^2 - (\sqrt{2} B d_d)^2}} \quad (3.32a)
\]

\[
2 \mu d_d = \frac{2 B^2 d_d}{\sqrt{(A_d v)^2 - (\sqrt{2} B d_d)^2}} \quad (3.32b)
\]

Let us remind us that \( \kappa \) and \( \mu \) must be positive. This is the reason why we introduced the prestress. Indeed, if \( \tau = 0 \), then we would have:

\[
\kappa = \frac{S_0}{d_v} - \frac{A^2}{\sqrt{(A_d v)^2 - (\sqrt{2} B d_d)^2}} \quad (3.33)
\]
which can become negative. Therefore, to ensure that $\kappa$ and $\mu$ are positive, we set:

\begin{align*}
\tau &= S_0 - \frac{2A^2d_v}{\sqrt{(Ad_v)^2 - (\sqrt{2}Bd_d)^2}} \quad (3.34a) \\
\kappa &= \frac{A^2}{\sqrt{(Ad_v)^2 - (\sqrt{2}Bd_d)^2}} > 0 \quad (3.34b) \\
\mu &= \frac{B^2}{\sqrt{(Ad_v)^2 - (\sqrt{2}Bd_d)^2}} > 0 \quad (3.34c)
\end{align*}

Then we have just two independent parameters for the behavior of the comparison composite, $\tau$ and $\mu$; since:

\begin{equation}
\frac{\kappa}{\mu} = \frac{A^2}{B^2} = \text{const.} \tag{3.35}
\end{equation}

and for the Drucker-Prager case (3.15):

\begin{equation}
\frac{\kappa}{\mu} = \frac{A^2}{B^2} = \frac{1}{\alpha_2^2} \tag{3.36}
\end{equation}

Finally, a substitution of the previous expressions in (3.29) yields the sought expression of $V$ for the hyperbolic criterion as a function of the independent parameters $\tau$ and $\mu$:

\begin{equation}
V_s = \left( \frac{B(S_0 - \tau)}{2A} \right)^2 \frac{1}{\mu} - \frac{1}{2\mu} - \frac{B^2}{4\mu} \tag{3.37}
\end{equation}

In the Drucker-Prager case (3.15), $V_s$ becomes:

\begin{equation}
V_s = (c_s - \alpha\tau)^2 \frac{1}{4\mu} \tag{3.38}
\end{equation}

### 3.3.4 Step 3: Stationarity of $\Pi^{\text{hom}}$

The third step consists in exploring the stationarity of $\Pi^{\text{hom}}$, that is Eq. (2.49). Note, however, that (3.35) reduces the degree of freedoms from three ($\kappa, \mu, \tau$) to two ($\mu, \tau$), whence:

\begin{equation}
\Pi^{\text{hom}} = \text{stat} [W_0(D_v, D_d) + \eta V_s] \tag{3.39}
\end{equation}

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Or explicitly:

\[
\frac{\partial \Pi^{\text{hom}}}{\partial \mu} = \frac{\partial \kappa}{\partial \mu} \frac{\partial \mathcal{W}_0}{\partial \mu} + \frac{\partial \mathcal{W}_0}{\partial \mu} + \eta \frac{\partial \mathcal{V}_s}{\partial \mu} = 0 \quad (\text{3.40a})
\]

\[
\frac{\partial \Pi^{\text{hom}}}{\partial \tau} = \frac{\partial \mathcal{W}_0}{\partial \tau} + \eta \frac{\partial \mathcal{V}_s}{\partial \tau} = 0 \quad (\text{3.40b})
\]

Using (3.28) and (3.37) in (3.40b) while making use of relation (3.35) yields:

\[
\frac{\partial \Pi^{\text{hom}}}{\partial \tau} = \frac{\mu}{\kappa} \kappa I_{D_v} + \frac{\tau}{\kappa^2} (\mu \kappa I - \kappa \eta) + \eta \frac{B^2}{A^2} \left( \frac{\tau - S_0}{2 \mu} \right) = 0
\]

\[
\tau = \frac{A^2 (2 \kappa I \mu D_v - \eta S_0)}{\eta A^2 - 2 \kappa I B^2}
\]

(3.41)

Then, substituting (3.41) into (3.40a) gives:

\[
\mu^2 = \frac{B^2}{A^2} \eta \left( \eta A^2 (S_0^2 - A^2) + \kappa I B^2 (2A^2 - S_0^2) \right)
\]

(3.42)

\[
\begin{aligned}
\frac{\partial \kappa^{\text{hom}}}{\partial \mu} &= \frac{\partial \kappa}{\partial \mu} \left( x_1 = \frac{A^2}{B^2}, \eta \right) = \mathcal{L}_I \\
\frac{\partial \mu^{\text{hom}}}{\partial \kappa} &= \frac{\partial \mu}{\partial \mu} \left( x_1 = \frac{A^2}{B^2}, \eta \right) = \mathcal{N}_I
\end{aligned}
\]

Then, making use of equations (3.28) and (3.37) and after simplification of the terms \( \mathcal{L}_I \) and \( \mathcal{N}_I \), equation (3.40a) becomes:

\[
\frac{\partial \Pi^{\text{hom}}}{\partial \mu} = \frac{1}{2} \kappa I D_v^2 + \mathcal{M}_I D_v^2 + \frac{\eta}{2} \left( \frac{B \tau}{A \mu} \right)^2 - \frac{K_I}{2} \left( \frac{B^2 \tau}{A^2 \mu} \right)^2 - \frac{\eta}{\mu^2} \left[ \left( \frac{B (S_0 - \tau)}{2A} \right)^2 - \frac{1}{2} B^2 \right] = 0
\]

Finally, plugging expression (3.41) for \( \tau \) into the last relation, we obtain the result (3.42).
Finally, using the values of \((\mu, \tau)\) corresponding to the stationarity of \(\tilde{\Pi}^{\text{hom}}\) in (3.39) provides the following estimate for \(\tilde{\Pi}^{\text{hom}}\):

\[
\tilde{\Pi}^{\text{hom}} = \frac{\eta K_1 B^2 S_0}{2K_1 B^2 - \eta A^2} D_v
- \frac{B}{A} \frac{\sqrt{\eta (\eta A^2 (S_0^2 - A^2) + K_1 B^2 (2A^2 - S_0^2)) (\eta K_1 A^2 D_v^2 + (2\eta A^2 - 4K_1 B^2) M_1 D^2_d)}}{(2K_1 B^2 - \eta A^2)}
\]

which can be recast in the more convenient form:

\[
\tilde{\Pi}^{\text{hom}} = \sum_0^{\text{hom}} D_v - \text{sign} (2K_1 B^2 - \eta A^2) \sqrt{(A^{\text{hom}})^2 D_v^2 + 2 (B^{\text{hom}})^2 D^2_d}
\]  

(3.44)

where:

\[
(A^{\text{hom}})^2 = \frac{\eta^2 B^2 K_1 (\eta A^2 (S_0^2 - A^2) + B^2 (2A^2 - S_0^2) K_1)}{(\eta A^2 - 2K_1 B^2)^2}
\]  

(3.45a)

\[
(B^{\text{hom}})^2 = \frac{\eta B^2 M_1 (\eta A^2 (S_0^2 - A^2) + B^2 (2A^2 - S_0^2) K_1)}{A^2 (\eta A^2 - 2B^2 K_1)}
\]  

(3.45b)

\[
\Sigma_0^{\text{hom}} = \frac{\eta B^2 K_1}{2K_1 B^2 - \eta A^2} S_0
\]  

(3.45c)

A comparison of (3.44) with (3.20) readily reveals that (3.44) is the \(\Pi\) function of a hyperbolic criterion, provided that \(2K_1 B^2 - \eta A^2 > 0\). In return, for \(2K_1 B^2 - \eta A^2 < 0\), we will see that \(\tilde{\Pi}^{\text{hom}}\) represents an elliptical strength criterion.

Last, in the Drucker-Prager case (3.15), the strength homogenization factors (3.45) simplify:

\[
\left(\frac{A^{\text{hom},1}}{c_s}\right)^2 = \frac{\eta^2 K_1 (\eta - \alpha_s^2 K_1)}{(\eta - 2\alpha_s^2 K_1)^2}
\]  

(3.46a)

\[
\left(\frac{B^{\text{hom},1}}{c_s}\right)^2 = \frac{\eta M_1 (\eta - \alpha_s^2 K_1)}{\eta - 2\alpha_s^2 K_1}
\]  

(3.46b)

\[
\Sigma_0^{\text{hom},1} = \frac{\eta \alpha_s K_1}{2K_1 \alpha_s^2 - \eta}
\]  

(3.46c)

and the class of criterion is now determined by the sign of \(X = 2\alpha_s^2 K_1 - \eta\): \(X > 0\) for an hyperbole, \(X < 0\) for an ellipse.
3.3.5 Step 4 & 5: Strength Criterion

There are different ways of obtaining the strength criterion.

Yield Design Approach

A rigorous approach makes use of the yield design definition (2.23), that is:

\[
\Sigma_m = \frac{1}{3} \text{tr} \Sigma = \frac{\partial \Pi^{\text{hom}}}{\partial D_v}; \quad \Sigma_d = \sqrt{S} = \frac{\partial \Pi^{\text{hom}}}{\partial D_d}
\]

(3.47)

where \( S = \Sigma - \Sigma_m \). Application to (3.44) gives:

\[
\Sigma_m = \Sigma^{\text{hom}}_0 - \frac{\text{sign} (2K_1 B^2 - \eta A^2) (A^{\text{hom}})^2}{\sqrt{(A^{\text{hom}})^2 D_v^2 + 2(B^{\text{hom}})^2 D_d^2}} D_v = \Sigma^{\text{hom}}_0 + \frac{(A^{\text{hom}})^2}{\Pi^{\text{hom}} - \Sigma^{\text{hom}}_0 D_v} D_v \quad (3.48a)
\]

\[
\Sigma_d = -\frac{2 \text{sign} (2K_1 B^2 - \eta A^2) (B^{\text{hom}})^2}{\sqrt{(A^{\text{hom}})^2 D_v^2 + 2(B^{\text{hom}})^2 D_d^2}} D_d = \frac{2(B^{\text{hom}})^2}{\Pi^{\text{hom}} - \Sigma^{\text{hom}}_0 D_v} D_d \quad (3.48b)
\]

Solving for \( D_v \) and \( D_d \) yields:

\[
D_v = \frac{\Sigma^{\text{hom}} - \Sigma^{\text{hom}}_0}{(A^{\text{hom}})^2 + (\Sigma^{\text{hom}} - \Sigma^{\text{hom}}_0) \Sigma^{\text{hom}}_0} \quad (3.49a)
\]

\[
D_d = \frac{\Sigma_d}{\sqrt{2B^{\text{hom}}}} \left( \frac{A^{\text{hom}}}{(A^{\text{hom}})^2 + (\Sigma^{\text{hom}} - \Sigma^{\text{hom}}_0) \Sigma^{\text{hom}}_0} \right)^2 \quad (3.49b)
\]

Finally, substituting (3.49) in (3.44) and eliminating \( \Pi^{\text{hom}} \) delivers after some transformations the sought strength criterion:

\[
\left( \Sigma_m = \frac{\partial \Pi^{\text{hom}}}{\partial D_v}; \quad \Sigma_d = \frac{1}{2} \frac{\partial \Pi^{\text{hom}}}{\partial D_d} \right) \in \partial \tilde{G}^{\text{hom}}
\]

(3.50)

\[
\left( \frac{\Sigma_m - \Sigma^{\text{hom}}_0}{(A^{\text{hom}})^2} + \frac{\Sigma_d}{\sqrt{2B^{\text{hom}}}} \right)^2 = 1
\]
Depending on the sign of the term \((B^{\text{hom}})^2\), the strength criterion can be either an ellipse \(((B^{\text{hom}})^2 > 0)\) or an hyperbole \(((B^{\text{hom}})^2 < 0)\), as displayed in Figure 3-5.

From its definition (3.45b), it is recognized that the sign of \((B^{\text{hom}})^2\) depends on the sign of \(\eta A^2 - 2K_I B^2\), that is:

\[
\text{sign} \left( (B^{\text{hom}})^2 \right) = \text{sign} (\eta A^2 - 2K_I B^2) = \begin{cases} 
-1 & \text{Hyperbolic Criterion} \\
0 & \text{Limit Parabola} \\
+1 & \text{Elliptical Criterion}
\end{cases} \tag{3.51}
\]
And in the Drucker-Prager case (3.46b):

\[
\eta - 2 \alpha_s^2 K_I \left( \frac{\kappa}{\mu} = \frac{1}{\alpha_s^2}, \eta \right) \begin{cases} 
< 0 & \text{Hyperbolic Criterion} \\
= 0 & \text{Limit Parabola} \\
> 0 & \text{Elliptical Criterion}
\end{cases}
\] (3.52)

**Short-Cut Solution**

A short-cut to the expression of the strength criterion is achieved by replacing \(D_v\) and \(D_d\) in the stationary conditions (3.40) by their expressions provided by the state equation (3.24) of the linear comparison composite:

\[
D_v = \frac{1}{\kappa_{\text{hom}}} \left( \Sigma_m - \frac{\kappa_{\text{hom}}}{\kappa} \tau \right) = \frac{1}{\mu} \kappa_{I} \left( \Sigma_m - \frac{B^2}{A^2} K_I \tau \right) 
\] (3.53a)

\[
D_d = \frac{1}{2\mu_{\text{hom}}} \Sigma_d = \frac{1}{2\mu} \mathcal{M}_I \Sigma_d
\] (3.53b)

This is the approach we prefer as a recipe (see Tab. 2.2). The two stationary conditions, (3.41) and (3.42), become:

\[
\frac{B^2}{2} 2 \Sigma_m - \tau \eta - S_0 \eta = 0
\] (3.54)

\[
\frac{A^2 K_I \Sigma_d^2 + 2 A^2 \mathcal{M}_I \Sigma_m^2 - 4 B^2 K_I \mathcal{M}_I \tau \Sigma_m + \eta B^2 K_I \mathcal{M}_I (\tau^2 + 2 S_0 \tau - S_0^2 + 2 A^2)}{4 A^2 K_I \mathcal{M}_I \mu^2} = 0
\] (3.55)

Solving (3.54) yields:

\[
\tau = \frac{2 \Sigma_m}{\eta} - S_0
\] (3.56)

Then, substituting (3.56) in (3.55) yields the sought macroscopic strength criterion (3.50).

**3.3.6 Pore Morphology Factors**

We are left with specifying the pore morphology factors, \(K_I\) and \(\mathcal{M}_I\), of the solid–void composite. Based on their definition (3.27), we refer to linear micromechanics.
Matrix–Pore Inclusion Morphology: Mori–Tanaka Scheme

Porous materials with a dominating matrix-pore inclusion morphology are well represented by the Mori-Tanaka scheme (MT) [72]. The matrix remains continuous for the entire solid concentration range \( \eta \in [0, 1] \); having thus a percolation threshold of \( \eta_0 = 0 \). Considering the Drucker-Prager case (3.36), the linear upscaling model gives (see Appendix A, Eq. (A.57)):

\[
\begin{align*}
K_{mt} &= \frac{\kappa_{\text{hom}}}{\mu} = K_I \left( \frac{\kappa}{\mu} = \frac{1}{\alpha_s^2}, \eta, \eta_0 = 0 \right) = \frac{4\eta}{3(1 - \eta) + 4\alpha_s^2} \quad (3.57a) \\
M_{mt} &= \frac{\mu_{\text{hom}}}{\mu} = M_I \left( \frac{\kappa}{\mu} = \frac{1}{\alpha_s^2}, \eta, \eta_0 = 0 \right) = \frac{\eta (9 + 8\alpha_s^2)}{15 - 6\eta + (20 - 12\eta)\alpha_s^2} \quad (3.57b)
\end{align*}
\]

Perfectly Disordered Solid–Pore Morphology: Self–Consistent Scheme

Perfectly disordered porous materials, such as granular materials, are well captured by the polycrystal, or self consistent model of micromechanics, which originated independently from Hershey [54] and Kröner [59]. The model treats each phase, solid and pore, of the porous composite as a phase surrounded by the averaged composite, hence the self-consistent terminology. The model is characterized by a percolation threshold \( \eta_0 = 1/2 \), below which the solid particles loose continuity, and which is consistent with the random loose packing fraction of spheres [76]; whence its popularity in the micromechanical modeling of granular materials. The linear self-consistent scheme provides the following expressions for \( K_I \) and \( M_I \) (see Appendix A, Eqs. (A.62) and (A.63); also [29]):

\[
K_{sc} = K_I \left( \frac{\kappa}{\mu} = \frac{1}{\alpha_s^2}, \eta, \eta_0 = 0.5 \right) = \frac{4\eta M_{sc}}{4\alpha_s^2 M_{sc} + 3(1 - \eta)} \quad (3.58)
\]

\[
M_{sc} = M \left( \frac{\kappa}{\mu} = \frac{1}{\alpha_s^2}, \eta, \eta_0 = 0.5 \right) = \frac{1}{2} - \frac{5}{4} (1 - \eta) - \frac{3}{16\alpha_s^2} (2 + \eta) \quad (3.59)
\]

\[
+ \frac{1}{16\alpha_s^2} \sqrt{144 (\alpha_s^4 - \alpha_s^2) - 480\alpha_s^4 \eta + 400\alpha_s^2 \eta^2 + 408\alpha_s^2 \eta - 120\alpha_s^2 \eta^2 + 9 (2 + \eta)^2}
\]

Without difficulty we verify that \( K_{sc} = M_{sc} = 0 \) at the percolation threshold \( \eta = \varphi = \eta_0 = 1/2 \).

Application of (3.52) then yields the critical packing density at which the strength criterion
reaches the limit parabola separating the hyperbolic case from the elliptical:

$$\eta - \eta^{cr}(\alpha_s) \begin{cases} > 0 & \text{Hyperbolic Criterion} \\ = 0 & \text{Limit Parabola} \\ < 0 & \text{Elliptical Criterion} \end{cases} \quad (3.60)$$

For the Mori-Tanaka pore morphology, substituting (3.57a) in (3.52) yields:

$$0 < \eta_{mt}^{cr} = 1 - \frac{4}{3} \alpha_s^2 \leq 1 \quad (3.61)$$

where the lower bound corresponds to the limit \(\alpha = \sqrt{3/4} = 0.86603\) given by (3.5).

In return, for the self-consistent pore morphology, substituting (3.58) in (3.52) gives:

$$\frac{2}{3} < \eta_{sc}^{cr} = 1 - \frac{1}{2} \sqrt{81 + 432 \alpha_s^2 + 1216 \alpha_s^4 - (9 + 16 \alpha_s^2)} \leq 1 \quad (3.62)$$

It is worth noting the limit development \(\eta_{sc}^{cr} = 1 - \frac{4}{3} \alpha_s^2 + O(\alpha_s^3)\) = \(\eta_{mt}^{cr} + O(\alpha_s^3)\), which shows that morphology is the more important the higher the friction.

3.3.7 Validation

We cannot close this Section on the Level I strength homogenization without a comparison of our results with the some results available in the open literature.

Gurson's Hollow Sphere Model

The most famous macroscopic strength model of a porous material is Gurson's 1977 hollow sphere model for porous ductile metals made of a Von-Mises solid phase \[49\]. Based on homogenization method and on the kinematic approach of limit analysis, which is known to be an upper bound \[61\] (see also \[47\] \[99\]), Gurson's strength criterion reads:

$$F(\Sigma_m, \Sigma_d) = 2 (1 - \eta) \left( \cosh \left( \frac{\sqrt{3} \Sigma_m}{2 \epsilon_s} \right) - 1 \right) + \left( \frac{\Sigma_d}{\sqrt{2} \epsilon_s} \right)^2 - \eta^2 = 0 \quad (3.63)$$
Gurson’s hollow sphere morphology comes closest to the matrix-pore inclusion morphology represented by the Mori-Tanaka scheme (3.57). Furthermore, given the assumed frictionless nature of the solid phase in Gurson’s model, the comparison is made for the limit case \( \alpha_s \to 0 \), for which (3.50) on account of (3.61) is an ellipse, with (3.46):

\[
\left( \frac{A_{\text{hom}}}{c_s} \right)^2 = \eta \mathcal{K}_{\text{mt}} (\alpha_s = 0) = \frac{4\eta^2}{3(1 - \eta)} \\
\left( \frac{B_{\text{hom}}}{c_s} \right)^2 = \eta \mathcal{M}_{\text{mt}} (\alpha_s = 0) = \frac{3\eta^2}{5 - 2\eta} \\
\frac{\Sigma_{\text{hom}}}{c_s} = 0
\]

Figure 3-6 compares the results for \( \alpha \to 0 \) (Von Mises) with Gurson’s strength criterion. In this extreme case of a Von-Mises material, it can be shown that our approach is an upper bound when associated to the Mori-Tanaka scheme. Gurson’s function is also an upper bound for the particular class of microstructures described by Hashin’s Composite Sphere Assemblage (CSA), and it gives the exact solution for purely hydrostatic loads. The comparison thus reveals that the elliptical criterion improves Gurson’s upper bound for deviatoric loading. However, for purely hydrostatic loading, the elliptical criterion performs poorly, particularly for high packing densities \( \eta \to 0 \). This has been recognized by several researchers [9],[38], with the explanation that the chosen nonlinear homogenization approach approximates the nonlinear behavior of the hollow sphere as just one phase, which is a too-poor representation to capture local shear effects that develop in hydrostatic compression around the cavity of the hollow sphere. To fully appreciate the comparison, it is instructive to develop the ‘cosh’ in Gurson’s criterion (3.63) in a power series \( (\cosh(x) = 1 + \frac{1}{2}x^2 + O(x^4)) \). Then Gurson’s criterion becomes an elliptical strength criterion of the form (3.50) with (3.46), if we let:

\[
\mathcal{K}_g = \frac{4\eta}{3(1 - \eta)}; \quad \mathcal{M}_g = \eta
\]

Hence, while the predictive capabilities of the elliptical criterion are restricted to modest hydrostatic loading, the Mori-Tanaka scheme provides a better estimate for macroscopic deviatoric loading.
Figure 3-6: Comparison of our results (solid line) with Gurson's model (dotted line).
Barthelemy–Dormieux Homogenization Model

A second comparison is made with the strength homogenization model by Barthelemy and Dormieux [3] [38]. Based on the effective strain rate approach, the authors arrive at an elliptical strength criterion for a porous material composed of a Drucker-Prager solid phase and voids, with the following ellipse parameters:

\[
\begin{align*}
\left(\frac{A_{\text{hom}}}{c_s}\right)^2 &= \frac{\eta^3 K'_I}{(\eta - \alpha_s^2 K'_I)^2} \\
\left(\frac{B_{\text{hom}}}{c_s}\right)^2 &= \frac{\eta^2 M'_I}{\eta - \alpha_s^2 K'_I} \\
\left(\frac{\Sigma_{0\text{hom}}}{c_s}\right) &= \frac{\eta \alpha_s K'_I}{\alpha_s^2 K'_I - \eta}
\end{align*}
\] (3.66)

where \(K'_I = K_I (\alpha_s = 0), M'_I = M_I (\alpha_s = 0)\) are the pore morphology factors (3.27) evaluated for an incompressible solid \((\kappa \to \infty \leftrightarrow \alpha_s = 0)\). For a Mori-Tanaka morphology, it turns out that the homogenization expressions \(A_{\text{hom}}\) and \(\Sigma_{0\text{hom}}\) coincide, while there is some slight difference in the \(B_{\text{hom}}\) coefficient, due to the restriction of (3.66) to an almost incompressible solid. We removed this restriction through relation (3.35).

3.4 Level II – Homogenization

Following the multiscale thought model of shales (see Fig. 3-1), the Level II–homogenization deals with the homogenization of rigid inclusions embedded in the porous clay phase (matrix). The strength behavior of the porous clay phase follows the hyperbolic or the elliptical criterion (3.50), while the rigid inclusions are assumed to have an unbounded strength domain. In this homogenization, a particular attention will be paid to the interface condition between inclusions and matrix, by considering two limit cases: perfect adherence and slippery imperfect interface.

In this derivation we continue to follow in a step-to-step fashion the recipe outlined in Table 2.2.
3.4.1 Step 1: Strain Rate Energy Function $W_0(D)$ of the Porous Clay–Inclusion Composite

The first step consists in calculating the strain rate energy function $W_0(D)$.

Consider the Level II RVE subjected to a regular strain rate boundary (3.21). The linear comparison composite is composed of a the porous clay phase ($V_{pc}$) and rigid inclusions ($V_{inc}$), so that the heterogenous stress distribution in the two phases reads as:

$$\sigma(\bar{x}) = C(\bar{x}) : d(\bar{x}) + \tau(\bar{x})$$  \hspace{1cm} (3.67)

where $C(\bar{x})$ and $\tau(\bar{x})$ are respectively the stiffness and the eigenstress whose spatial distributions within the RVE are given by:

$$C(\bar{x}) = \begin{cases} C_{pc} = (3\kappa_{pc} I + 2\mu_{pc} K) & (V_{pc}) \\ \infty & (V_{inc}) \end{cases} \hspace{1cm} \tau(\bar{x}) = \begin{cases} \tau_{pc} = \tau_{pc} I & (V_{pc}) \\ 0 & (V_{inc}) \end{cases}$$  \hspace{1cm} (3.68)

where $C_{pc}$ and $\tau_{pc}$ are respectively the stiffness tensor and the prestress of the porous clay phase in the Linear Comparison Composite.\(^3\) With the help of linear micromechanics results for a solid (with prestress) and rigid inclusions, the macroscopic stress state equation is found:

$$\Sigma = C_{hom,II} : D + T^{II}$$  \hspace{1cm} (3.69)

where $C_{hom,II}$ and $T^{II}$ are respectively the Level II homogenized stiffness tensor and the Level II macroscopic prestress (see Appendix A, Eqs. (A.114) and (A.133)):

$$C_{hom,II} = C(\bar{x}) : A(\bar{x}) = 3\kappa^{II} I + 2\mu^{II} K$$  \hspace{1cm} (3.70a)

$$T^{II} = \tau(\bar{x}) : A(\bar{x}) = T^{II}_m = \tau_{pc} I$$  \hspace{1cm} (3.70b)

\(^3\)Note that the Linear Comparison Composite (LCC) at level II is a priori independent of the LCC at level I. In order to avoid any confusion, we therefore note the input stiffness and the input prestress in (3.70) by $C_{pc}$ and $\tau_{pc}$ and not by $C_{hom,I}$ and $T^I$ given by (3.25).
By analogy with (3.27), we write the homogenized moduli $\kappa^{\text{hom}} = \kappa^{II}$ and $\mu^{\text{hom}} = \mu^{II}$ in the form:

\begin{align}
\kappa^{II} &= \mu_{pc} \mathcal{K}_{II} \left( \frac{\kappa_{pc}}{\mu_{pc}}, f_{inc} \right) \\
\mu^{II} &= \mu_{pc} \mathcal{M}_{II} \left( \frac{\kappa_{pc}}{\mu_{pc}}, f_{inc} \right)
\end{align}

(3.71a)
(3.71b)

where $\mathcal{K}_{II}$ and $\mathcal{M}_{II}$ are solid-inclusion morphology factors, that account for the type of morphology (Mori-Tanaka, Self-Consistent, etc.), the interface condition (perfect adherence, slippery imperfect interface), and the inclusion volume fraction $f_{inc}$. They will be specified later on.

For the porous-clay solid – rigid inclusion composite, the strain rate energy function $W_0(D)$ reads (see Appendix A, Eq. (A.133)):

$$W_0(D) = \frac{1}{2} D : C^{\text{hom}, II} : D + T^{II} : D$$

(3.72)

That is, in the isotropic case:

$$W_0(D_v, D_d) = \frac{1}{2} \kappa^{II} D_v^2 + \mu^{II} D_d^2 + T^{II}_{d,v} D_v$$

$$= \frac{1}{2} \mu_{pc} \mathcal{K}_{II} D_v^2 + \mu_{pc} \mathcal{M}_{II} D_d^2 + \tau_{pc} D_v$$

(3.73)

where $D_v = \text{tr}(D)$ and $D_d = \sqrt{\Delta : \Delta}$ with $\Delta = D - \frac{1}{3} D \cdot 1$.

### 3.4.2 Step 2: $V$ Function (for an Elliptical Criterion)

The second step consists in determining the $V$ function (Eq. (2.50)) for the (porous clay) solid phase ($V = 0$ for rigid inclusions):

$$V_{pc} = \text{stat} \{ \pi_{pc}(d) - \omega_{pc}(d) \}$$

(3.74)

where:

- The support function $\pi_{pc}(d)$ of the porous clay phase is given by expression (3.44), which
we recall:

\[ \pi_{pc}(d) = \tilde{H}_{\text{hom},l}(D \to d) = S'_0 d_v - \text{sign}(X) \sqrt{(A'_I d_v)^2 + 2 (B'_I d_d)^2} \] (3.75)

where \( X = 2 \alpha^2 \kappa_I - \eta \) distinguishes the hyperbolic \((X > 0)\) from the elliptical case \((X < 0)\); and \( S'_0, A'_I, B'_I \) are the Level I homogenization results (3.46):

\[ A'_I = A^{\text{hom},l}; \quad B'_I = B^{\text{hom},l}; \quad S'_0 = S^{\text{hom},l}_0 \] (3.76)

- The strain rate energy function of the porous clay solid phase is akin to (3.30):

\[ \omega_{pc}(d) = \frac{1}{2} \kappa_{pc} d_v^2 + \mu_{pc} d_d^2 + \tau_{pc} d_v \] (3.77)

In the derivation of the expression of the \( V \) function associated with an hyperbolic criterion (3.37), we started with (3.14) which includes a minus sign but in which \( B^2 > 0 \). Therefore, in the case where the strength criterion of the porous phase is an hyperbole, we need to adapt result (3.37) to the form (3.75) by replacing \((B'_I)^2\) by \(-(B'_I)^2\); that is:

\[ V_{pc}(X > 0) = \frac{1}{2} \frac{(B'_I)^2}{\mu_{pc}} - \left( \frac{B'_I (S'_0 - \tau_{pc})}{2 A'_I} \right)^2 \frac{1}{\mu_{pc}} \] (3.78)

together with (analogous to (3.35)):

\[ \frac{\kappa_{pc}}{\mu_{pc}} = - \text{sign}(X) \left( \frac{A'_I}{B'_I} \right)^2 = \text{const.} \]

where \(- \text{sign}(X)\) accounts for the fact that \((B'_I)^2 < 0\) in the hyperbolic case \((X > 0)\).
Consider next the elliptical case, \( X < 0 \). Applying the stationarity condition to the \( V_{pc} \) function defined by (3.74), (3.75) and (3.77) yields:

\[
\frac{\partial V_{pc}}{\partial d_v} = 0 \Rightarrow \kappa_{pc}d_v + \tau_{pc} = S_0' + \frac{(A')^2}{\sqrt{(A'd_v)^2 + (\sqrt{2}B'd_d)^2}}
\]

(3.79a)

\[
\frac{\partial V_{pc}}{\partial d_d} = 0 \Rightarrow 2\mu_{pc}d_d = \frac{2(B')^2}{\sqrt{(A'd_v)^2 + (\sqrt{2}B'd_d)^2}}
\]

(3.79b)

For the same reason as in the hyperbolic case (positive \( \kappa_{pc} \) and \( \mu_{pc} \)), we need to use a prestress, and let:

\[
\tau_{pc} = S_0'
\]

(3.80a)

\[
\kappa_{pc} = \frac{(A')^2}{\sqrt{(A'd_v)^2 + (\sqrt{2}B'd_d)^2}}
\]

(3.80b)

\[
\mu_{pc} = \frac{-\text{sign}(X)(B')^2}{\sqrt{(A'd_v)^2 + (\sqrt{2}B'd_d)^2}}
\]

(3.80c)

These relations ensure not only that \( \kappa_{pc} \) and \( \mu_{pc} \) remain positive, but also – akin to (3.35):

\[
\frac{\kappa_{pc}}{\mu_{pc}} = -\text{sign}(X) \left( \frac{A'}{B'} \right)^2 = \text{const.}
\]

(3.81)

The expression for \( V_{pc} \) for the elliptical case thus becomes:

\[
V_{pc}(X < 0) = \frac{1}{2} \frac{(B')^2}{\mu_{pc}}
\]

(3.82)

### 3.4.3 Step 3–5: Stationarity of \( \bar{\Pi}_{\text{hom}} \) – Hyperbolic Strength Criterion

We now turn to exploring the stationarity of \( \bar{\Pi}_{\text{hom}} \), that is Eq. (2.49). The hyperbolic case is first considered, \( X > 0 \). There are two degrees of freedom, \( \mu_{pc} \) and \( \tau_{pc} \):

\[
\bar{\Pi}_{\text{hom}} = \text{stat}_{\mu_{pc}, \tau_{pc}} [W_0(D_v, D_d) + (1 - f_{inc}) V_{pc}]
\]

(3.83)
Using expressions (3.73) and (3.78), stationarity w.r.t. $\tau_{pc}$ yields:

$$\frac{\partial \Pi_{\text{hom}}}{\partial \tau_{pc}} = D_v - (1 - f_{inc}) \frac{(B')^2}{2 (A')^2 \mu_{pc}} (\tau_{pc} - S_0^I) = 0$$

$$\Downarrow$$

$$\tau_{pc} = S_0^I + 2\mu_{pc} \left( \frac{A'}{B'} \right)^2 \frac{D_v}{(1 - f_{inc})}$$

(3.84)

Similarly, the stationarity condition w.r.t. $\mu_{pc}$ gives (analogous to (3.40a)):

$$\frac{\partial \Pi_{\text{hom}}}{\partial \mu_{pc}} = \frac{1}{2} K_{II} D_v^2 + M_{II} D_d^2 + \frac{(1 - f_{inc})}{(\mu_{pc})^2} \left[ \left( \frac{B^I(S_0^I - \tau_{pc})}{2A^I} \right)^2 - \frac{1}{2} (B^I)^2 \right] = 0$$

(3.85)

Finally, replacing in the stationary conditions (3.84) and (3.85) the macroscopic strain rates, $D_v$ and $D_d$, by their expressions provided by the linear elastic stress equation of state of the linear comparison composite (3.69); that is:

$$D_v = \frac{1}{K_{II}} (\Sigma_m - \tau_{pc})$$

$$D_d = \frac{1}{2\mu_{II}} \Sigma_d$$

(3.86a, b)

We obtain the sought Level II macroscopic strength criterion for the rigid inclusion – porous clay composite defined by an hyperbolic strength criterion:

$$X > 0 \quad \frac{(\Sigma_m - \Sigma_0^I)^2}{(A^I)^2} + \frac{(\Sigma_d/\sqrt{2})^2}{(B^I)^2} = 1$$

(3.87)

where:

$$(A^I)^2 = 2 (A')^2 + (B')^2 K_{II} (1 - f_{inc})$$

(3.88a)

$$(B^I)^2 = (B')^2 M_{II} (1 - f_{inc})$$

(3.88b)

$$\Sigma_0^I = S_0^I = \Sigma_0^I$$

(3.88c)
Since \((B^{II})^2 < 0\), it is found that the solid-inclusion composite, whose solid phase obeys to a hyperbolic criterion \(((B^I)^2 < 0)\), is always governed by a hyperbolic criterion.

Finally, for the Drucker-Prager case, combining (3.45) and (3.76) with (3.46) allows expressing the hyperbole parameters in functions of the Level I pore morphology factors \((K, M_I)\) and the Level II solid-inclusion morphology factors \((Ku_I, Mil)\):

\[
\left( \frac{A^{II}}{c_s} \right)^2 = \frac{\eta (\eta - \alpha_s^2 K_I) (2\eta K_I + M_I (\eta - 2\alpha_s^2 K_I) (1 - f_{inc}) K_{II})}{(\eta - 2\alpha_s^2 K_I)^2} \quad (3.89a)
\]

\[
\left( \frac{B^{II}}{c_s} \right)^2 = \frac{\eta M_I (\eta - \alpha_s^2 K_I) (1 - f_{inc}) M_{II}}{\eta - 2\alpha_s^2 K_I} \quad (3.89b)
\]

\[
\frac{\Sigma_{0}^{II}}{c_s} = -\frac{\alpha_s \eta K_I}{\eta - 2\alpha_s^2 K_I} \quad (3.89c)
\]

We remind ourselves, that in the hyperbolic case:

\[
X > 0 \Leftrightarrow \eta > 2\alpha_s^2 K_I \quad (3.90)
\]

### 3.4.4 Step 3–5: Stationarity of \(\tilde{\Pi}^{hom}\) – Elliptical Strength Criterion

Consider next the case of the porous clay phase following an elliptical criterion, \(X < 0\). Due to relation (3.80a), which fixes the value of \(\tau_{pc}\), the stationary condition depends only on \(\mu_{pc}\) as sole degree of freedom; that is:

\[
\frac{\partial \tilde{\Pi}^{hom}}{\partial \mu_{pc}} = \frac{1}{2} K_{II} D_o^2 + M_{II} D_d^2 - (1 - f_{inc}) \frac{(B^I)^2}{2 (\mu_{pc})^2} = 0 \quad (3.91)
\]

Then, a substitution of (3.86) in (3.91) leads to the sought strength criterion:

\[
X < 0 \quad \frac{(\Sigma_m - \Sigma_0^{II})^2}{(A^{II})^2} + \frac{(\Sigma_d/\sqrt{2})^2}{(B^{II})^2} = 1 \quad (3.92)
\]

78
\begin{align*}
(A^{II})^2 &= (B^{II})^2 \mathcal{K}_I (1 - f_{mc}) \\
(B^{II})^2 &= (B^{II})^2 \mathcal{M}_I (1 - f_{mc}) \\
\Sigma_0^{II} &= S_0 = \Sigma_0^{\text{hom, I}}
\end{align*}

Since \((B^{II})^2 > 0\) in the elliptical case, and thus \((B^{II})^2 > 0\), it turns out that the composite strength domain of the composite, whose solid phase is described by an elliptical strength domain, is also always an ellipse.

Finally, combining Level I and Level II homogenization results, i.e. (3.45) and (3.93), yields the following expressions for the ellipse parameters:

\begin{align*}
\left(\frac{A^{II}}{c_s}\right)^2 &= \frac{\eta (\eta - \alpha_2^2 \mathcal{K}_I) \mathcal{M}_I}{\eta - 2\alpha_2^2 \mathcal{K}_I} (1 - f_{mc}) \mathcal{K}_{II} \\
\left(\frac{B^{II}}{c_s}\right)^2 &= \frac{\eta (\eta - \alpha_2^2 \mathcal{K}_I) \mathcal{M}_I}{\eta - 2\alpha_2^2 \mathcal{K}_I} (1 - f_{mc}) \mathcal{M}_{II} \\
\frac{\Sigma_0^{\text{hom}}}{c_s} &= -\frac{\alpha_s \eta \mathcal{K}_I}{\eta - 2\alpha_2^2 \mathcal{K}_I}
\end{align*}

\subsection{3.4.5 Level II – Solid-Inclusion Morphology Factors}

We are left with specifying the Level II solid-inclusion morphology factors \((\mathcal{K}_{II}, \mathcal{M}_{II})\) which are defined by (3.71), and which depend on the morphology (Mori-Tanaka vs. Self-Consistent) and on the interface conditions. To start with, let us specify the \(\kappa_{pc}/\mu_{pc}\) ratio in (3.71) from (3.81) and the Level I homogenization results (3.46) for the Drucker-Prager case:

\[ \beta = \frac{\kappa_{pc}}{\mu_{pc}} = -\text{sign}(X) \frac{(A^{II})^2}{(B^{II})^2} = \frac{\eta \mathcal{K}_I}{\mathcal{M}_I |\eta - 2\mathcal{K}_I \alpha_2^2|} > 0 \]

The determination of the solid-inclusion morphology factors \((\mathcal{K}_{II}, \mathcal{M}_{II})\) then consists of using (3.95) in linear upscaling solutions that consider the morphology (Mori-Tanaka vs. Self-Consistent) and the interface conditions. We thus distinguish the following four cases:
Matrix–Inclusion Morphology with Perfect Interface Adherence

Inclusions embedded in a matrix, are well represented by the Mori-Tanaka scheme. In the case of a perfect adherence, linear homogenization theory provides the following estimate (see Appendix A, Eq. (A.58)):

\[
\kappa_{tt}^{mt,A} = \frac{13\beta + 4f_{inc}}{3(1-f_{inc})} \quad (3.96a)
\]

\[
\mathcal{M}_{tt}^{mt,A} = \frac{1}{4} \left( \frac{9f_{inc} + 6}{(1-f_{inc})(2+\beta)} \right) (8f_{inc} + 12) \quad (3.96b)
\]

Matrix–Inclusion Morphology with Slippery Interface Imperfections

If the inclusion-matrix interface permits a free tangential slip, then the Mori-Tanaka scheme provides the following estimate of the solid-inclusion morphology factors (see Appendix A, Eq. (A.60)):

\[
\kappa_{tt}^{mt,L} = \frac{13\beta + 4f_{inc}}{3(1-f_{inc})} \quad (3.97a)
\]

\[
\mathcal{M}_{tt}^{mt,L} = \frac{1}{4} \left( \frac{9f_{inc} + 15}{(5-2f_{inc})(2+\beta)} \right) (8f_{inc} + 24) \quad (3.97b)
\]

Disordered Solid–Inclusion Morphology with Perfect Interface Adherence

A disordered morphology of the porous clay phase with inclusions, in which neither phase is recognized as a distinct matrix phase, is well represented by the self-consistent scheme. In the case of perfect adherence, the solid-inclusion morphology factors read (see Appendix A, Eqs. (A.64) and (A.65)):

\[
\kappa_{tt}^{sc,A} = \frac{1}{18} \left( \frac{1}{(1-f_{inc})(1-2f_{inc})} \right) \left( \frac{(18 + 15f_{inc}^2 - 42f_{inc})\beta + 4f_{inc}(3 - f_{inc})}{(18 + 15f_{inc}^2 - 42f_{inc})\beta + 4f_{inc}(3 - f_{inc})} \right) \quad (3.98)
\]

\[
\mathcal{M}_{tt}^{sc,A} = \frac{1}{24} \left( \frac{1}{1-2f_{inc}} \right) \left( \frac{(15f_{inc} - 6)\beta + (12 - 4f_{inc})}{(15f_{inc} - 6)\beta + (12 - 4f_{inc})} \right) \quad (3.99)
\]

where \( f_{inc} < 0.5 \) is the volume fraction of the rigid inclusions with perfect interface adherence.
Disordered Solid–Inclusion Morphology with Slippery Interface Imperfections

If the interface permits a free tangential slip, the solid-inclusion morphology factors read for a self-consistent morphology (see Appendix A, Eqs. (A.66) and (A.67)):  

\[
K_{II}^{sc,L} = \frac{1}{18} \frac{1}{(1-f_{inc})(2-3f_{inc})} \left( (3(8f_{inc}^2 - 23f_{inc} + 12))\beta + 8f_{inc}(3-2f_{inc}) \right) \\
\]

\[
\ldots + f_{inc} \sqrt{9(8f_{inc} - 5)^2 \beta^2 + (720 - 1392f_{inc} + 528f_{inc}^2) \beta + 64(2f_{inc} - 3)^2} \right) \\
\]

\[
K_{II}^{sc,R} = \frac{1}{24} \frac{1}{2 - 3f_{inc}} \left( (24 - 16f_{inc}) - (15 - 24f_{inc}) \beta \right) \\
\]

\[
\ldots + \sqrt{9(8f_{inc} - 5)^2 \beta^2 + (720 - 1392f_{inc} + 528f_{inc}^2) \beta + 64(2f_{inc} - 3)^2} \right) \\
\]

where \(f_{inc} < 2/3\) is the volume fraction of the rigid inclusions with slippery boundary conditions.

The Level II homogenization is then complete.

3.4.6 Validation

To validate the solution, we compare our result in the hyperbolic case (3.88) to the solution of Barthelemy and Dormieux for the case of rigid inclusions embedded in a Drucker-Prager matrix, characterized by its cohesion, \(c\), and friction coefficient, \(\alpha\) [4]. Their solution reads:

\[
\frac{\Sigma_d}{\sqrt{2}} + \alpha_{BD} \left( \Sigma_m - \frac{c}{\alpha} \right) = 0 \\
\]

where, using the Mori-Tanaka scheme with perfect adherence conditions:

\[
\alpha_{BD}^{hom,mt,A} = \alpha \sqrt{\frac{1 + \frac{3}{2}f_{inc}}{1 - \frac{4}{3}f_{inc}\alpha^2}} \\
\]

and with free tangential slip:

\[
\alpha_{BD}^{hom,mt,L} = \alpha \sqrt{\frac{(1 + \frac{3}{5}f_{inc})(1 - f_{inc})}{(1 - \frac{4}{5}f_{inc}\alpha^2)(1 - \frac{2}{5}f_{inc})}} \\
\]

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To compare this solution with our Level II result (3.87) with (3.88), we let:

\[
\begin{align*}
(B^I)^2 &= -\alpha^2 (A^I)^2 \\
S_0^I &= \frac{c}{\alpha} \\
(A^I)^2 \rightarrow 0^+ 
\end{align*}
\]

Equation (3.87) thus becomes:

\[
\frac{\Sigma_d}{\sqrt{2}} + \alpha \sqrt{\frac{\mathcal{M}_{II} (1 - f_{inc})}{2 - \alpha^2 \mathcal{K}_{II} (1 - f_{inc})}} \left( \Sigma_m - \frac{c}{\alpha} \right) = 0
\]

which correspond to a Drucker-Prager criterion with homogeneous friction coefficient:

\[
\alpha^{\text{hom}} = \alpha \sqrt{\frac{\mathcal{M}_{II} (1 - f_{inc})}{2 - \alpha^2 \mathcal{K}_{II} (1 - f_{inc})}}
\]

This limit case compares fairly well with Barthelemy and Dormieux’s solution based on the effective strain rate theory. Indeed, in the case of perfect adherence, the ratio between the two solutions is always comprised between 0.90 and 1, and in the case of free tangential slip, it is comprised between 0.98 and 1.

### 3.5 Chapter Summary

In this Chapter we put to work the linear comparison composite theory for the strength homogenization of shale viewed as a multiscale composite. The outcome is a two-scale strength homogenization model which is sufficiently flexible to account for different pore morphologies, interface conditions, etc. In a forward application (morphology known), this model requires as input the following parameters:

- At level ‘0’, the strength properties of the composite constituents, namely the cohesion $c_s$ and the friction angle $\alpha_s$ of the elementary building block of shales.
- At level ‘I’, the packing density $\eta$ of the porous clay composite, respectively the clay porosity $\varphi = 1 - \eta$.
- At level ‘II’, the silt inclusion volume fraction, $f_{inc}$. 

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We thus arrive at reducing the complexity of shale's strength behavior to a four-parameter strength model. This highly reductionist approach will turn out most useful in applications, in which those parameters are known from strength tests, mineralogy and porosity measurements. In return, as we will see in the next part of this report, the approach lends itself readily for an inverse application that aims at determining shale fundamental mechanical properties and morphology from micro- and/or macroscopic strength data. This will be illustrated in the remainder of this report for a particular strength test: the indentation hardness test.
Part III

Indentation Hardness Analysis
Chapter 4

Brief Introduction to Indentation Testing and Analysis

The general goal of indentation analysis is to translate the results of an indentation test (typical an experimental force-indentation depth curve) into meaningful mechanical properties of the indented material. This part deals with such an indentation analysis, namely with the indentation analysis of the strength properties of the constituents of an heterogenous material obtained from indentation hardness measurements at the scale of the composite. It is composed of two chapters. This Chapter provides an introduction to the indentation technique and indentation analysis. It focusses in particular on the self-similarity of the indentation test, the extraction of the indentation modulus and the indentation hardness from an indentation test, and on a dimensional analysis of the relevant quantities involved in an indentation in an heterogeneous material, which at a scale smaller than the indentation depth is composed of different phases. This is the situation we consider in the next chapter, in which we use the expressions of the homogenized strength criteria derived in Chapter 3 for indentation analysis. In fact, by simulating the indentation experiment in this homogenized medium, hardness-packing density scaling are derived which make the link between the strength properties of the constituents, morphology parameters and hardness as measured in an indentation test.
4.1 The Indentation Test

The underlying idea of a modern indentation experiment is that the contact response of a material can be used to characterize its bulk mechanical properties (for a historical review, see Table 4.1). In such a test, a hard tip of known geometry and mechanical properties is pressed into the sample and both the load and the displacement are recorded. The resulting curve, load vs. displacement, gives a fingerprint of the material and can be used to extract some of its mechanical properties, namely elastic, strength/hardness and creep properties. The term nanoindentation refers to an indentation experiment in which the typical indentation depth is less than a micron (< $10^{-6}$ m). While the use of instrumented nanoindentation has been extensively studied in the past two decades (for recent reviews, see [75],[21]), the tools have been limited, until recently, to either homogeneous samples or to layered samples (thin films) whose thicknesses are previously known (see e.g. [78]). Recently developed and refined techniques, however, have extended the application of nanoindentation to heterogeneous composite materials [26], [29], [28], [102], [10].

4.1.1 Description of the Experiment

The typical nanoindentation device is sketched in Figure 4-1. Although this experiment is conceptually simple, its actual implementation is a real challenge as it involves different ultra high precision devices. In a general way, a nanoindenter has to carry out 3 main functions: position the sample under the indenter tip, control the displacement of the tip and apply a load. As nanoindentation operates at very small depth, all of these functions have to be performed with a very high precision.

The positioning of the sample is performed using both an optical microscope and a motor driven XY stage controlled by a computer. The sample is first positioned under the microscope in order to observe it and determine the indentation coordinates. Then, a calibrated translation moves the sample under the indenter tip in order to proceed to indentation. The strongest zoom available on our machine is 100 times and the resolution of the work table is 1 μm. It is possible to repeat the experiment and obtain a "map" of the mechanical properties of the sample by performing a grid of nanoindentations [27] [28]. In that case, we must make sure that

\footnote{Some elements of this presentation are inspired from Cornell University website: http://www.nanoindentation.cornell.edu}
**Historical Background: Indentation Test**

The concept of hardness can be found as early as in the 18th century in the work of Réaumur (1683–1757) and Mohs (1773–1839) as a means of material classification. The first example of engineering application of indentation methods appeared in the work of the Swedish engineer Brinell, published in a 1900 international congress in Paris [17]. Pushing a small ball of hardened steel or tungsten carbide against the surface of the specimen, Brinell empirically correlated the shape of the resulting permanent impression (indentation) with the strength of the metal alloys. The merits of Brinell's proposal were quickly appreciated by contemporaries: Meyer (1908), O'Neill (1944) and Tabor (1951) suggested empirical relations to transform indentation data into meaningful mechanical properties [98].

In contrast to hardness measurements, much of the theoretical foundations of elastic indentation analysis originates from Heinrich Hertz' 1882 classical paper: *On the contact of elastic solids* [55]. In this article Hertz studied the influence of the contact force holding a set of lenses on their optical properties. However, in contrast to the empirical approaches relating an residual imprint to strength properties, elastic contact mechanics requires a continuous measurement of the indentation force and indentation depth.

This idea lead Tabor and coworkers to conceptualize indentation techniques that would monitor the indentation depth [98] [92]. The implementation of depth sensing indentation techniques down to the nanoscale appears to have developed first in the former Soviet Union from 1950 to 1980. This instrumented indentation approach received considerable attention world-wide in the late 1980s when Doerner and Nix [36] and Oliver and Pharr [74] identified it for analysis and estimation of mechanical properties of materials such as microelectronic thin films for which few other experimental approaches were available. Today, nanoindentation constitutes a very promising experimental technique for the investigation of nanomechanical properties of metals, ceramics, polymers, and composites.

Table 4.1: Background: Historical Background on indentation technique (adapted from [27])
the indents are sufficiently spaced in order to avoid any interaction between two neighboring tests.

Most of the nanoindentation machines are load controlled. The displacements are only measured and not controlled. This choice implies that the force actuator must provide a precise force that is not perturbed by a small change in displacement, which is often called a "soft" load control. There are different methods to achieve this high precision load actuation. The most famous is electromagnetic actuation. The principle is the same as the one of a speaker: a coil of wire is placed in a permanent magnet. When an electrical signal is applied to the coil, a magnetic field is created and interacts with the permanent magnet, generating a mechanical force. This method of actuation is reliable over a wide range of displacement and loads. Other methods of load actuation include electrostatic actuation and spring actuation.

There are also different methods for the measurement of the displacement. Capacitive displacement gages can measure very accurately the variation of the distance between its two planes (resolution close to $1\,\text{Å} = 10^{-10}\text{m}$). However, their disadvantage lies in their very short range of operation. Others method are based on optical properties such as optical lever methods. They utilize a laser beam whose deflection is measured by a differential photodiode device.
and gives a measure of the displacement. Such devices achieve resolutions comparable to an interferometer and are also used in most Atomic Force Microscopes (AFM).

4.1.2 Experimental Issues

As it is the case for many experimental techniques, several factors can disrupt the accuracy of the nanoindentation measurement. It is important to be aware of them in order to minimize their importance and account for them in the analysis of the results. One frequent issue is the machine compliance. That includes the non zero compliance of the different parts of the machine as well as, for instance, the compliance of the load actuator. These aspects have to be quantified and must be subtracted from the load-displacement data.

Another important issue emanating from the machine is the thermal drift phenomenon. This is primarily due to the large size of the machine parts compared to the measured indentation depths and to the heat generated by the different electronic devices. In order to minimize it, a temperature control system is usually associated to the nanoindentation machine. Mechanical drift may also be felt due to surrounding vibrations and justifies the presence of an important damping system under the machine.

Finally, the most important issue linked to the sample is its roughness. This aspect becomes all the more important when it comes to granular materials like shale. The situation is sketched in Figure 4-2. The problem appears when the typical size of the roughness is comparable to the indentation depth (case b). In this case, we cannot define a real contact elevation for the tip and the analysis based on an indentation in a half space is not valid anymore. The indentation depth must be much greater than the typical size of the roughness (case a), which represents a lower bound for the experimental indentation depth. Different techniques have been developed in order to minimize this problem [70] [58].

4.1.3 Derived Indentation Properties

The indentation test consists of making contact between a sample and an indenter tip of known geometry and mechanical properties, followed by a continuously applied and recorded change in load, \( P \), and depth, \( h \). Typical tests consist of a constantly increasing load, followed by a short hold and then a constant unloading; a \( P - h \) curve is reported (Fig. 4-3). The analysis
Figure 4-2: Importance of surface roughness. This figure was generated from real AFM imaging of a shale sample after polishing.

Figure 4-3: A typical indentation curve in a force driven indentation test [Courtesy of C. Bobko].
of the $P - h$ curve proceeds by applying a continuum scale model to condense the indentation response into two indentation properties; indentation modulus, $M$,

$$M \overset{\text{def}}{=} \sqrt{\frac{\pi}{2}} \frac{S}{\sqrt{A_c}}$$  \hfill (4.1)

and indentation hardness, $H$:

$$H \overset{\text{def}}{=} \frac{P}{A_c}$$  \hfill (4.2)

where $S = \frac{dP}{dh}$ is the (measured) initial slope of the unloading branch of the $P - h$ curve, $P$ is the (measured) maximum indentation load, and $A_c$ is the projected contact area of the indenter on the sample surface (Fig. 4-4), which is a priori an unknown of the contact problem.

Fortunately, there exist indirect methods for its determination as a function of the (measured) maximum indentation depth, $h_{\text{max}}$. The most employed method is due to Oliver and Pharr [74], and is based on the determination of the contact height $h_c$ from the elastic contact solution:

$$h_c = h_{\text{max}} - \epsilon \frac{P_{\text{max}}}{S}$$  \hfill (4.3)

where $(h_{\text{max}}, P_{\text{max}}, S)$ are all measured quantities, while $\epsilon = 0.72, 0.75$ and 1, for cone-, sphere- and flat-punch-geometry, respectively. Finally, the indenter contact area $A_c$ is calculated using the area function of the indenter, which in the case of a perfect Berkovich indenter reads:

$$A_c(h_c) = 24.5 \ h_c^2$$  \hfill (4.4)

### 4.2 Indentation Analysis

The aim of indentation analysis is to link the indentation quantities $(M, H)$ to meaningful material properties of the indented material.
Figure 4-4: Conical indentation in a porous material, composed of a solid phase and pore space: (a) matrix-porosity morphology; (b) perfectly disordered, polycrystal morphology [adapted from [20]].
4.2.1 Indentation Modulus

Definition (4.1) of the indentation modulus finds its theoretical foundation in the works of Boussinesq and Hertz. Boussinesq’s stress and displacement solution of an elastic half space loaded by a rigid axisymmetric indenter [16], was subsequently extended for conical and cylindrical indenter geometry [64][43]. Together with Hertz’s elastic contact solution of two spherical surfaces with different radii and elastic constants [55], this work forms the basis of much experimental and theoretical work in indentation analysis based on contact mechanics. In the isotropic case, \( M \) reduces to the plane-stress modulus [43][91]:

\[
M = \frac{E}{1-\nu^2} = \frac{C_{11}^2 - C_{12}^2}{C_{11}} \tag{4.5}
\]

where \( E \) is the Young’s modulus, \( \nu \) the Poisson’s ratio; \( C_{11} = C_{1111} \) and \( C_{12} = C_{1122} \) are the two stiffness coefficients describing the isotropic elastic behavior of the half-space. In the case of anisotropic elasticity, things are more complicated as the indentation modulus depends on the direction of indentation w.r.t. the material’s symmetry axis. General solutions for this problem are quite involving [106] [103] [104] [96] [105], but can be simplified into explicit relations for specific material symmetries with high accuracy. For instance, in the case of a transverse isotropic elastic half space, with \( x_3 \) being the material symmetry axis, the indentation moduli \( M_i = M(x_i) \) obtained from indentation in the principal material axis \( x_i \) are linked to the five independent elasticity constants by [39], [51],[32]:

\[
M_3 = M(x_3) = 2\sqrt{\frac{C_{11}C_{33} - C_{13}^2}{C_{11}}} \left( \frac{1}{C_{44}} + \frac{2}{\sqrt{C_{11}C_{33} + C_{13}}} \right)^{-1} \tag{4.6}
\]

\[
M_1 = M(x_1) = M(x_2) \approx \sqrt{\frac{C_{11}C_{11}^2 - C_{12}^2}{C_{33}}} M_3 \tag{4.7}
\]

where we employ Voigt notation \( C_{11} = C_{1111}, C_{12} = C_{1122}, C_{13} = C_{1133}, C_{33} = C_{3333}, C_{44} = C_{2323} = C_{1313} \).
4.2.2 Indentation Hardness

As the hardness incorporates plasticity phenomena, the indentation analysis is a much more complex problem than the elastic contact problem which is well served by Hertz-type contact mechanics. The non linear nature of the constitutive relations, as well as the increased number of material properties required to describe the material behavior, complicates the derivation of analytical solutions. As a result, much of our knowledge of the importance of plasticity in indenter contact problem has been derived through experimentation and more recently through finite element simulations. Various researchers have proposed procedures in which the experimental $P - h$ response can be used to derive elasto-plastic properties such as the Young's modulus $E$, the initial yield stress $Y$ for a Von Mises type material and the strain hardening exponent $[36], [79], [46], [107], [31], [23]$. Experimental data have demonstrated that analysis of indentation data provides reasonable estimates of the elastic modulus and hardness of the indented material, provided that the contact area is measured or calculated accurately.

4.3 Self-Similarity of the Indentation Test

4.3.1 Indenter Shapes

Any indenter shape must meet two requirements: it must be made of a hard material (typically diamond), and it must have a precise geometry at the length scale of a few nanometers. The most common shapes of indenters are sharp pyramidal or spherical (Fig. 4-5). Spherical indenters provide a smooth transition between elastic and elasto-plastic contact [7], and are commonly used for larger scales as the evolution of the contact area with depth is rapidly evolving.

The Berkovich tip is the standard nanoindentation tip. It has a three-sided pyramidal shape with total angle from one edge to the opposite side of 142.35°. The Cube Corner indenter tip is also a 3 sided pyramidal tip but has total angle of 90° degrees. In contrast, the Vickers tip is a four sided pyramidal tip with a semi-vertical angle of 68°, which has the same area-to-depth ratio as a Berkovich tip. However, because it is harder to make four planes intersect at one point than it is with three planes, the Vickers tip cannot be as precisely manufactured as the Berkovich tip, and is therefore less used in nanoindentation.
4.3.2 Self-Similarity Properties

One key feature of the analysis of pyramidal or conical indentation is the self-similarity of Hertz-type contact problems. This self-similarity allows one to scale the force-indentation depth solution by simple renormalization of one known solution. For instance, Galanov [42] used the explicit form of the Boussinesq solution for a concentrated load to generate indentation solutions in the case of an isotropic material, and Borodich [13] applied a similar approach to the anisotropic case. The conditions under which frictionless indentation contact problems possess classical self-similarity are as follows [14]:

1. The shape of the indenter is described by a homogeneous function whose degree is greater or equal to unity. Using a Cartesian coordinate system $Ox_1x_2x_3$ whose origin $O$ is at the indenter tip and $x_3$ is the orientation of the indentation, the shape of the indenter is defined by:

$$x_3 = f(x_1, x_2)$$  \hspace{1cm} (4.8)

$$f(\lambda x_1, \lambda x_2) = \lambda^d f(x_1, x_2) \begin{cases} \text{for any } \lambda > 0 \\ \text{with } d \geq 1 \end{cases}$$  \hspace{1cm} (4.9)

---

This Section is inspired by the presentation of the topic by Constantinides [27].
Here \( d \) is the degree of the homogeneous function \( f \); in particular \( d = 1 \) for a cone and \( d = 2 \) for the elliptic paraboloid considered by Hertz. Axisymmetric indenters can be described by monomial functions of the form (first introduced by Galin, according to Borodich and Keer [15]):

\[
f(x_1 = r \cos(\phi), x_2 = r \sin(\phi)) = B(\phi) r^d
\]

where \( B(\phi) \) describes the height of the indenter at point \((\phi, r = 1)\). For a conical indenter having a semi vertical angle \( \theta \), \( B = \cot(\theta) \). For a spherical indenter of radius \( R \), \( d = 2 \) and \( B = 1/(2R) \). The previous expression was recently extended to indenters of non-axisymmetrical shape, such as pyramidal indenters that are frequently employed in depth-sensing indentation tests [14]. For a three-sided pyramid, \( d = 1 \), and making use of triple symmetry:

\[
B(\phi) = \cot(\theta) \sin\left(\frac{\pi}{6} + \phi\right)
\]

where \( \theta \) is the angle in vertical cross-sections. For a Berkovich indenter, having a face angle of \( 115.13^\circ \), \( \theta = 65.3^\circ \).

2. The constitutive relationships are homogeneous functions of degree \( \kappa \) with respect to the strain tensor \( \varepsilon_{ij} \):

\[
\mathcal{F}(\lambda \varepsilon_{ij}) = \lambda^\kappa \mathcal{F}(\varepsilon_{ij})
\]

Evidently, a linear elastic law satisfies this relation, since \( \kappa = 1 \); as does any nonlinear secant elastic formulation of the form \( \sigma = C(\varepsilon) : \varepsilon \), for which the secant elastic stiffness tensor satisfies:

\[
C(\lambda \varepsilon) = \lambda^{\kappa-1} C(\varepsilon)
\]

A similar reasoning applies to a yield design formulation of the form (2.51), for which according to (2.11) and (2.52), \( \kappa \to 0 \).

Then provided the homogeneity of material properties and that the operator \( \mathcal{F} \) remains the same for any depth of indentation, the whole load-displacement curve in a depth sensing test
can be scaled by [14]:

\[
\frac{P_1}{P_2} = \left(\frac{h_1}{h_2}\right)^{\frac{2+\kappa(d-1)}{d}}; \quad \frac{h_1}{h_2} = \left(\frac{A_{c1}}{A_{c2}}\right)^{\frac{d}{2}}
\]

(4.14)

where \(A_c\) is the projected contact area, which appears to be not affected by the constitutive relation factor \(\kappa\). Furthermore, from a straightforward application of (4.2) and (4.14), the hardness scales with the indentation depth according to:

\[
\frac{H_1}{H_2} = \left(\frac{h_1}{h_2}\right)^{\frac{\kappa(d-1)}{d}}
\]

(4.15)

Hence, in the case of conical and pyramidal indenters, we find that the load-displacement relation is scaled by \(P \propto h^2\) and that the hardness is constant over the loading process and does not depend on the indentation depth. This justifies \textit{a posteriori} the definition of the hardness and its status as a material property.

Finally, as noted here before, cones and three-sided pyramidal indenter tips have the same \(d = 1\) degree of the homogeneous function. It is, therefore, common practice to assimilate, in the indentation analysis, the original three-sided pyramid with an equivalent cone of revolution, such that the projected contact area w.r.t. the indentation depth is the same:

\[
A(h) = C_1 h^2 = \pi (h \tan \theta)^2 \Rightarrow \tan \theta = \sqrt{\frac{C_1}{\pi}}
\]

(4.16)

where \(C_1\) is a constant characterizing the specific pyramidal indenter and \(\theta\) is the equivalent semi-apex cone angle. For the Berkovich indenter, for which \(C_1 = 24.56\) (see Eq.(4.4)) the equivalent cone has a semi-apex angle \(\theta = 70.32^\circ\).

4.4 Multi-Scale Indentation Analysis of Heterogeneous Materials

The indentation technique has been extensively used to characterize homogeneous materials such as metals or polymers. The indentation analysis is based on considering the sample as an infinite half space composed of a monophasic homogeneous material. This methodology however, is currently restricted to monolithic systems, and little has been reported for indentation
on heterogeneous composite materials, a category composing the majority of solids, including shales (see Fig. 3-1). The application of indentation analysis to porous materials faces several challenges. Porous materials are by nature heterogeneous, as they are composed of a solid phase and a pore space. This heterogeneity may itself influence the indentation response, and may eventually lead to a break of the self-similarity of the indentation test, if the pore size is of a similar order as the indentation depth $h$. In return, if the pore size is much smaller than the indentation depth, which is the case in most natural composites dominated by nanoporosity, then an indentation test provides access to the homogenized composite properties of the porous material. The challenge of the indentation analysis then is to extract from the indentation data, for instance hardness $H$, the strength properties of the solid phase. The focus of this Section is to extend the realm of indentation analysis to indentation in such random composites, as opposed to thin-films. In order to facilitate the indentation analysis in this case, we start with a dimensional analysis.

### 4.4.1 Dimensional Analysis

Dimensional analysis is a powerful tool very often used in sciences to understand physical situations involving several quantities. The fundamental idea is that physical laws do not depend on arbitrarily chosen basic units of measurement. This basic idea leads to the so-called II-theorem which has been attributed to Buckingham [18]. It allows one to identify key ratios in the problem and to reduce the number of arguments in the different mathematical expressions.

In this light, consider an indentation test of a rigid conical indenter (half-cone angle $\theta$, indentation depth $h$) into an infinite half-space composed of a cohesive-frictional porous material (Fig. 4-4), similar to the Level I homogenization situation of shales (Fig. 3-1). The indented material is a two-phase composite composed of a solid phase and a pore space. The behavior of the solid phase is defined by the stiffness $C_{ijkl}$ and the cohesive-frictional solid strength parameters, cohesion $c_s$ and friction coefficient $\alpha_s$. In addition, in a first approximation, the overall response of the porous composite depends on the solid concentration or packing density, $\eta = 1-\varphi$, where $\varphi$ is the porosity, and the morphology at the microscale, expressed in this model by the packing density percolation threshold associated with $\eta_0$ ($\eta_0 = 0$ corresponds to a matrix-pore morphology associated with the Mori- Tanaka scheme, $\eta_0 = 0.5$ corresponds to a granular
morphology associated with the self-consistent scheme, see Section 3.3.6). The question we here address is how those parameters affect the experimentally measurable indentation hardness (4.2).

For the dimensional analysis, we consider the two dependent variables in the contact problem [21] that define the hardness, namely indentation force \( P \) and projected contact area \( A_c \):

\[
P = f(h, \theta, C_{ijkl}, c_s, \alpha_s, \eta, \eta_0) \quad (4.17a)
\]

\[
A_c = f(h, \theta, C_{ijkl}, c_s, \alpha_s, \eta, \eta_0) \quad (4.17b)
\]

Application of the \( \Pi \)-theorem [18] to (4.17) yields the dimensionless relations:

\[
\frac{P}{c_s h^2} = \Pi_P \left( \theta, \frac{C_{ijkl}}{c_s}, \alpha_s, \eta, \eta_0 \right) \quad (4.18a)
\]

\[
\frac{A_c}{h^2} = \Pi_{A_c} \left( \theta, \frac{C_{ijkl}}{c_s}, \alpha_s, \eta, \eta_0 \right) \quad (4.18b)
\]

A substitution of (4.18) in (4.2) readily yields a new invariant, the hardness-to-solid cohesion ratio:

\[
\frac{H}{c_s} = \frac{\Pi_P}{\Pi_{A_c}} = \Pi_H \left( \theta, \frac{C_{ijkl}}{c_s}, \alpha_s, \eta, \eta_0 \right) \quad (4.19)
\]

The dimensionless relation \( \Pi_H \) confirms that the hardness does not depend on the indentation depth. This is due to the absence of any other length scale in the infinite half-space cohesive-frictional model, including characteristic material lengths, such as the Burgess vector that characterize dislocations.

Empirical relations between hardness and material properties can be traced back to the work of the Swedish Engineer Brinell (1849–1925) who correlated the strength of metal alloy with the shape of the permanent impression left by a small ball of hardened steel or tungsten carbide on the material surface [17] (see Table 4.1). From slip-line field solution for indentation in a rigid cohesive plastic solid by a frictionless rigid wedge, Tabor suggested a hardness (\( H \)) vs. yield strength (\( Y \)) relationship of the form \( H/Y = 3 \) [97]. This relation got under scrutiny by several researchers for elastic-perfectly plastic solids (see discussion in [57]) and more recently for work-hardening materials (see discussion in [21]). In particular, for elastoplastic cohesive solids, it was shown from comprehensive finite element simulations of conical indentation \( \theta = 68^\circ \), that
the $H/Y$-ratio for cohesive materials, for which $(C_{ijkl}/Y)^{-1} \to 0$, comes close to Tabor’s 1948 suggestion (noting that the yield strength $Y$ relates to the cohesion $c_s$ of the Von-Mises solid by $Y = \sqrt{3}c_s$) [21]:

$$\frac{H}{Y} = \frac{1}{\sqrt{3}} \Pi_H \left( \theta = 68^\circ, \frac{C_{ijkl}}{Y} \to \infty, \alpha_s = 0, \eta = 1 \right) \simeq 2.8$$  \hspace{2cm} (4.20)

The assumption $(C_{ijkl}/Y)^{-1} \to 0$ comes close to the rigid-plastic assumption of yield design approaches which can be found early on in the indentation literature. For instance, Lockett [63] and Chitkara and Butt [22] developed yield design solutions for conical indentations in cohesive rigid-plastic solids (without and with friction at the indenter-material interface). More recently, using the upper bound theorem of yield design, Ganneau et al. [45],[100] [44] developed a dual indentation approach which allows the determination of cohesion and friction of a Mohr-Coulomb solid (Eq. (3.2)) from the dependence of the hardness-to-cohesion ratio on the cone angle:

$$\frac{C_{ijkl}}{c_s} \to \infty; \frac{H}{c_s} = \Pi_H' \left( \theta, \mu, \eta = 1 \right)$$  \hspace{2cm} (4.21)

where $\mu = \tan \varphi$ is the Coulomb friction coefficient.

Very recently, Cariou et al. [19],[20] incorporated into the indentation analysis the strength properties of the solid’s constituents ($c_s$ and $\alpha$), the porosity ($\varphi = 1 - \eta$) and the microstructure (percolation threshold $\eta_0$):

$$\frac{C_{ijkl}}{c_s} \to \infty; \frac{H}{c_s} = \Pi_H \left( \theta, \alpha_s, \eta, \eta_0 \right)$$  \hspace{2cm} (4.22)

This was achieved based on yield design assumption, and an elliptical strength criterion derived from Barthelemy and Dormieux’s effective strain rate approach (i.e. Eq. (3.50) with (3.66)).

To our knowledge, the hyperbolic case has not yet been considered for the derivation of hardness-packing density scaling relations of the form (4.22); nor the addition of rigid inclusions with different interface conditions at level II, as derived in Chapter 3. This is in short the focus of the next Chapter. More precisely, by means of a multi-scale yield design approach, we develop such solutions which incorporate into the indentation analysis the strength properties of the solid’s constituents ($c_s$ and $\alpha$), the Level I porosity ($\varphi = 1 - \eta$) and its microstructure (per-
colation threshold \( \eta_0 \), the Level II rigid inclusions (volume fraction \( f_{inc} \)) and their morphology and interface conditions (see Section 3.4.5):

\[
\frac{H}{c_s} = \Pi_H (\theta, \alpha_s, \eta, \eta_0, f_{inc}, f_0)
\] (4.23)

This will be achieved by means of a numerical yield design approach.

4.4.2 Yield Design Based Multi-Scale Indentation Analysis

The developments here below are based on continuum indentation analysis based on yield design theory, and assumes the existence of a representative volume element (RVE) of a characteristic length scale \( L \), which satisfies the scale separability condition:

\[
d \ll L \ll h
\] (4.24)

The characteristic size of the microstructure \( d \) is defined by the size of the porosity at Level I and by the size of the inclusions at Level II. The indentation depth \( h \) which is the only relevant length scale of the indentation operation in the infinite half space (which by its very nature has no length scale), characterizes the order of magnitude of the variation of the position vector \( \mathbf{z} \), and therefore determines the characteristic length scale of the application of the tools of differential calculus necessary for indentation analysis.

The work rate provided by a rigid conical indenter to an infinite half-space is:

\[
\delta W = P \hat{h} = \int_{A_M} \mathbf{T}(\mathbf{n}) \cdot \mathbf{U} da = \int_{\Omega} \mathbf{\Sigma} : \mathbf{D} d\Omega
\] (4.25)

where \( \hat{h} \) is the indentation rate, \( A_M = A_c / \sin \theta \) is the contact area of the cone mantel with the material (\( A_c \) being the projection of this surface on the \( z \)-axis); \( \mathbf{T}(\mathbf{n}) = \mathbf{\Sigma} \cdot \mathbf{n} \) is the stress vector on \( A_M \) oriented by the unit outward normal \( \mathbf{n} \) (positive outward to the material domain; i.e. in a cylinder coordinate frame \( \mathbf{n} = -\cos \theta \mathbf{e}_r + \sin \theta \mathbf{e}_z \)); and \( \mathbf{U} \) is the velocity field of the material on \( A_M \). Furthermore, from an application of the divergence theorem, the external work rate is equal to the work realized by the (Cauchy) stress \( \mathbf{\Sigma} \) along the strain rate \( \mathbf{D} \) in the half-space \( \Omega \). The stress field \( \mathbf{\Sigma} = \mathbf{\Sigma}(\mathbf{z}) \) is statically admissible, satisfying equilibrium and the
(assumed) frictionless contact condition at the indenter-material interface $A_M$, where all shear stresses are zero, \( \Sigma (\mathbf{n}) = \Sigma n; \) hence:

\[
\begin{align*}
(a) \quad & \Sigma = \Sigma^T; \ \text{div} \Sigma = 0; \  \mathbf{[T]} = [\Sigma \cdot \mathbf{n}] = 0 \\
(b) \quad & -P_2 = \int_{A_M} T (\mathbf{n}) \ da \\
(c) \quad & \forall (r, z) \in A_M (\mathbf{t} \cdot \mathbf{n} = 0); \quad \left\{ \begin{array}{l}
\mathbf{t} \cdot T(\mathbf{n}) = \frac{1}{2} (\Sigma_{zz} - \Sigma_{rr}) \sin 2 \theta + \Sigma_{r} \cos 2 \theta = 0 \\
\mathbf{n} \cdot T(\mathbf{n}) = \Sigma_{rr} \sin^2 \theta + \Sigma_{zz} \cos^2 \theta - \Sigma_{r} \sin 2 \theta 
\end{array} \right.
(d) \quad & \forall r \geq a; z = 0: T (\mathbf{n}) = 0
\end{align*}
\]

(4.26)

where superscript $T$ stands for transpose and $a$ is the contact radius.

Furthermore, application of yield design theory to (4.25) comes to assume that the material system in $\Omega$, at plastic collapse, has exhausted, in response to the prescribed force $P$, its capacities, (i) to develop stress fields $\Sigma = \Sigma (x)$ that are both statically compatible in the sense of (4.26) with the external loading and compatible with the local strength domain $G (x)$ of the constitutive materials; and (ii) to store the externally supplied work rate (4.25) into recoverable elastic energy. As a consequence, the work rate $\delta W$ is entirely dissipated in the material bulk. Those two conditions are captured by the following dual definitions of the materials strength capacity (see Section 2.1):

\[
\begin{align*}
(a) \quad & \Sigma \in G (x) \iff F (\Sigma) \leq 0 \\
(b) \quad & \Pi (\mathbf{D}) = \sup (\Sigma : \mathbf{D}; \ F (\Sigma) \leq 0) \geq 0 \\
(c) \quad & \Sigma \in \partial G (x) \iff \Sigma = \frac{\partial \Pi (\mathbf{D})}{\partial \mathbf{D}}
\end{align*}
\]

(4.27)

Herein, $F (\Sigma) = 0$ is the yield function which defines the boundary $\partial G (x)$ of the strength domain of the material system in continuous material sub-domains, and which is convex w.r.t.
In turn, $\Sigma : D$ represents the maximum dissipation capacity the material can develop in the material bulk for the solution fields $(\Sigma, U)$. This dissipation capacity is expressed by the dissipation function or support function $\Pi(D)$ which is defined on the set of symmetric second-order tensors $D$, and which is convex w.r.t. $D$. In particular, $D$ is the solution strain rate field in continuous material sub-domains, which is kinematically compatible with the velocity field $U$ and compatible with the normality rule of plastic flow of the material:

$$D = \frac{1}{2} (\text{grad } U + T \text{grad } U) = \lambda \frac{\partial F(\Sigma)}{\partial \Sigma}$$ (4.28)

where $\lambda$ is the plastic multiplier. For the indentation test in an infinite half-space, a velocity field $U = U(x)$ is kinematically admissible, if it satisfies the zero-velocity boundary conditions at infinity. Furthermore, the frictionless contact condition at the indenter-material interface a priori permits a tangential slip (without dissipation), while the normal velocity $U \cdot n$ is the one of the rigid indenter:

$$\begin{cases} 
(a) & \forall (r, z) \in A_M; \ U \cdot n = -\dot{h} \sin \theta \\
(b) & (r, z) \rightarrow \infty; \ U = 0
\end{cases}$$ (4.29)

Finally, if we remind ourselves that $\Pi(\lambda D) = \lambda \Pi(D)$ $(\forall \lambda \in \mathbb{R}^+)$, the contact condition (4.29(a)) implies that the yield design solution $P\dot{h}$ is proportional to $\dot{h}$. In other words, $\dot{h}$ is a dummy variable, which we set equal to $\dot{h} = 1$, so that (4.25) yields the sought expression that links the hardness (4.2) to the dissipation capacity of the material half-space:

$$H = \frac{P}{A_c} = \frac{1}{A_c} \int_{\Omega} \Sigma : D d\Omega; \ \dot{h} = 1$$ (4.30)

The classical limit theorems of yield design approach the actual dissipation capacity (4.30) by a lower and an upper bound estimate. The lower estimate is based on statically and plastically admissible stress fields $\Sigma'$ satisfying (4.26) and (4.27(a)), and underestimates the dissipation capacity of the material. This provides a lower bound estimate $H^-$ of the hardness:

$$H^- \leq H = \frac{1}{A_c} \sup_{F(\Sigma' \cdot D) \leq 0} \int_{\Omega} \Sigma' : D d\Omega; \ \dot{h} = 1$$ (4.31)

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The upper bound approach is based on kinematically and plastically admissible strain rate fields $D'$ satisfying (4.28) and (4.29), and provides an upper bound estimate $H^+$ of the hardness:

$$
H = \frac{1}{A_e} \inf_{\{D\prime\}} \int_{\Omega} \Pi (D') \, d\Omega \leq H^+; \quad \hat{h} = 1
$$

(4.32)

Finally, for the evaluation of the hardness-to-strength property relation all comes down to estimating the strength domain of the heterogeneous material. Thanks to the scale separability condition (4.24) we can separate the scale of the RVE from the one of its constituents, i.e. the solid phase and the pore space at level I and the rigid inclusions at level II. All what it thus takes is to use the estimates of respectively the homogenized strength criterion (3.50) and the support function (3.44) derived in Chapter 3 with the appropriate morphology factors in relations (4.31) and (4.32) to obtain the sought hardness–material properties–morphology relations (4.23). The conceptual simplicity of the procedure, however, belies its complexity. This is why we resort in the next Chapter to the tools of advanced numerical limit analysis to solve this problem.

4.5 Chapter Summary

The application of nanoindentation to porous materials, like shale, has provided the poromechanics community with a new versatile tool to test in situ phase properties and structures of porous materials that cannot be recapitulated ex situ in bulk form. But it requires a rigorous indentation analysis to translate indentation data into meaningful mechanical properties. This is not an easy task. The way how we propose to address this challenge is by means of a multiscale yield design approach to indentation analysis, which recognizes the separation of scale condition. The chosen approach aims at translating recent progress in non-linear micromechanics based on micro-yield design theory into a workable model for indentation analysis based on macro-yield design theory. The input to this approach is the micro-yield design theory shown in previous chapters that provide analytical expressions of the homogenized strength domain of the material at different scales, Level I and Level II, in functions of constituent properties $(c^a, \alpha)$ and microstructure parameters $(\eta, \eta_0, f_{inc}, f_0)$. The macro-yield design theory embeds these micro-macro relations into the evaluation of the indentation hardness. The implementation of this approach is the focus of the next chapter.
Chapter 5

Hardness–Microstructure Relations

This Chapter develops hardness–microstructure relations for shales of the form (4.23):

\[
\frac{H}{c_s} = \Pi_H (\theta, \alpha_s, \eta, \eta_0, f_{inc}, f_0)
\]  

(5.1)

This will be achieved for the Berkovich indenter shape \((\theta = 70.32^\circ)\) using an advanced computational implementation of the yield design approach together with the homogenized strength criteria for Level I (solid-pore composite) and for Level II (porous solid–rigid inclusion composite). The computational platform is due to Prof. Lavinia A. Borges [11], [85], and the results presented in this Chapter are to a large extent the outcome of a fruitful collaboration with Prof. Borges during her sabbatical stay at MIT in 2006/07. Borges’ computational approach is first presented, followed by a presentation of the simulation results and a validation. Finally, from the simulation results, we derive hardness–packing density scaling relations for different pore morphologies (Level I) and solid-inclusion morphologies (Level II), that will turn out useful for day-to-day indentation testing of shale materials.

5.1 Limit Analysis Solver

This Section presents the main characteristics of the nonlinear optimization algorithm we employ to determine the hardness–to–cohesion relation (5.1). The algorithm and its implementation was realized by Prof. Lavinia A. Borges from the Departamento e Programa de Engenharia
5.1.1 Problem Formulation

Borges' algorithm is neither based on a strict lower bound approach nor on a strict upper bound approach in the sense of yield design theory. Instead, it aims at directly finding a numerical estimate of the stress and velocity fields which are the solution of the limit analysis problem. In fact, the approach employs both stresses and velocities as degrees of freedom, and subjects them to the following conditions:

1. The stress field $\Sigma$ satisfies the weak form of the equilibrium condition $\text{div} \Sigma = 0$, as expressed by the theorem of virtual work rate. For the indentation test as defined by (4.25), this condition reads:

\[ P\vec{h} = \int_{\Omega} \Sigma : D(\vec{U}^*) \ d\Omega \quad \forall \vec{v}^* \in \mathcal{K} \]  

(5.2)

where $D(\vec{U}^*)$ is the strain rate tensor. The velocity field $\vec{U}^*$ is kinematically admissible in the sense of (4.29); and belongs to the following set of kinematically admissible velocity fields of the indentation test:

\[ \mathcal{K} = \left\{ \vec{U}(x) \text{ s.t. } \begin{cases} \forall x \in A_M \quad \vec{U}(x) \cdot \vec{n} = -\vec{h} \sin(\theta) \\ \vec{U}(x) = 0 \quad \text{for } |x| \to \infty \end{cases} \right\} \]

(5.3)

1. The stress field satisfies the strength criterion; that is:

\[ F(\Sigma) = \frac{(\Sigma_m - \Sigma_0^{\text{hom}})^2}{(A^{\text{hom}})^2} + \frac{(\Sigma_d/\sqrt{2})^2}{(B^{\text{hom}})^2} - 1 \leq 0 \quad \forall x \in \Omega \]

(5.4)

where $f(\Sigma)$, in our case, can be an elliptical or a hyperbolic strength criterion, depending on the sign of $(B^{\text{hom}})^2$.

2. The strain rate $D(\vec{U}^*)$ obeys an associated flow rule in the sense of (4.28):

\[ D(\vec{U}^*) = \frac{1}{2} \left( \text{grad} \ \vec{U}^* + T \text{grad} \ \vec{U}^* \right) - \lambda \frac{\partial F(\Sigma)}{\partial \Sigma} \quad \forall x \in \Omega \]

(5.5)
where the plastic multiplier $\dot{\lambda}$ obeys to:

$$\dot{\lambda} \geq 0; \quad F(\Sigma) \leq 0; \quad \dot{\lambda} F(\Sigma) = 0 \quad \forall \Sigma \in \Omega$$  \hspace{1cm} (5.6)

### 5.1.2 Finite Element Formulation

The implementation of the approach requires on the one side the discretization of the material domain $\Omega$, and on the other hand an efficient formulation to solving the constraint conditions. The first objective is readily achieved by using the classical procedures of finite element analysis (see e.g. [6]). The infinite half-space $\Omega$ is replaced by a finite domain $\Omega'$, and $\Omega'$ is discretized by finite elements. Both the velocity field $U^*$ and the stress field $\Sigma$ are discretized by means of finite element interpolations, replacing the continuum fields by discrete nodal vectors: a $n$-dimensional vector $v$ with $n$ denoting the number of degrees of freedom in the discrete model, a $q$-dimensional vector of stress components $T$ for all nodes in the finite element mesh. Using the classical notation of displacement-based finite element formulation which is here applied to the velocity formulation, the components of the strain rate tensor are given by:

$$D = Bv$$  \hspace{1cm} (5.7)

where $B$ is the strain rate–velocity matrix (equivalent to the strain-displacement matrix in the FEM). The plastic functions $F(T)$ are represented as a vector-valued function of plastic admissibility constraints in each Gauss point of each finite element. Similarly, the loading is represented by a vector $PF$ such that:

$$PF^T v = Ph; \quad \forall v \in K$$  \hspace{1cm} (5.8)

which is the discretized form of (5.2).

It is assumed that all rigid motions are ruled out by prescribed kinematic constraints; therefore, the kernel of matrix $B$ contains only the null velocity vector. The discrete optimality conditions representing the limit analysis problem after using suitable finite element interpolations are:

$$\Psi(K) = 0 \; ; \; f(T) \leq 0 \; ; \; \dot{\lambda} \geq 0$$  \hspace{1cm} (5.9)
with

$$
\Psi (X) = \begin{bmatrix} B^T T - P F \\ B_v - \dot{\lambda} \nabla f(T) \\ G(T) \dot{\lambda} \end{bmatrix}, \quad X = \begin{bmatrix} T \\ v \\ P \\ \dot{\lambda} \end{bmatrix}
$$

(5.10)

and $G(T) = \text{diag}(f_j(T))$. $\dot{\lambda}$ is the vector of plastic multipliers.

5.1.3 Algorithmic Formulation

The solution of the (5.9) is done in an iterative fashion. The goal of the algorithm is to find a vector $X$ such that each equation is enforced, allowing for a certain infinitesimal error. The static and plastic admissibility condition of the stress field is always enforced in the algorithm, by means of the following convergence criterion:

$$
\left\| B_v - \dot{\lambda} \nabla f(T) \right\|_\infty \leq \varepsilon_D \left\| B_v \right\|_\infty \\
\dot{\lambda}_j \leq \varepsilon_\lambda \left\| \dot{\lambda} \right\|_\infty \quad \text{if} \quad f_j(T) \leq \varepsilon f_j(0) \\
\dot{\lambda}_j \geq -\varepsilon_\lambda \left\| \dot{\lambda} \right\|_\infty
$$

(5.11)

A discretization of the problem must be done in order to handle it numerically. An adaptive mesh procedure automatically generated several reference mesh suited for different parameters of the second order strength criterion.

Each iteration of the algorithm consists in using a Newton-type algorithm associated with the set of all equalities in the optimality conditions (5.9), followed by a step relaxation and stress scaling in order to preserve plastic admissibility. A search direction $d_X^0$ is determined by a Newton iteration, that is, an increment for $X$ is estimated by solving:

$$
J(X) d_X^0 = -\Psi(X)
$$

(5.12)
where \( J(\lambda) = \nabla \Psi(\lambda) \) in the case of the Newton algorithm. Thus:

\[
\begin{bmatrix}
-H & B & 0 & -\nabla f \\
B^T & 0 & -F & 0 \\
0 & -F^T & 0 & 0 \\
-\Lambda \nabla f^T & 0 & 0 & -G
\end{bmatrix}
\tag{5.13}
\]

with:

\[
\Lambda = \text{diag} \left( \lambda_j \right) 
\tag{5.14}
\]

\[
H = \sum \lambda_j \left( \nabla^2 f_j + \epsilon M \right) 
\tag{5.15}
\]

where \( \epsilon M \) is a small perturbation in order to avoid the Hessian singularity, present in the hyperbolic case.

Assume that the weak equilibrium condition (5.8) is exactly satisfied for the present values of \( T \) and \( P \). Then expand (5.12) to obtain a linear system of equations whose variables are the stress increments \( d^o_p \), the load factor increment \( d^o_p \), and the new estimates for \( y \) and \( \lambda \), denoted \( y^0 \) and \( \lambda^0 \). The solution of this system leads to:

\[
d^o_p = \frac{1}{E} \cdot \hat{\nu}^o, \quad \nu^o = d^o_p \cdot \hat{\nu}
\tag{5.16}
\]

where the vector \( \hat{\nu} \) is determined as the solution of the linear system:

\[
K \hat{\nu} = F
\tag{5.17}
\]

while matrix \( K \) assembles the contributions of each finite element:

\[
K = B^T D^e p B
\tag{5.18}
\]

with:

\[
D^e p = H^{-1} - Q W^{-1} Q^T, \quad Q = H^{-1} \nabla f, \quad W = \nabla f^T H^{-1} \nabla f - \Lambda^{-1} G
\tag{5.19}
\]
Once $\mathbf{u}^0$ is obtained, the new estimates for $d_T^0$ and $\lambda^0$ are given by:

$$
\lambda^0 = W^{-1}Q^T B\mathbf{u}_0^0, \quad d_T^0 = D^{ep} B\mathbf{u}_0^0
$$

(5.20)

An updating performed at the end of each iteration enforces that $\lambda_j$ is strictly positive. Under this condition, it can be proven that the symmetric matrix $W$ is positive definite and the symmetric matrix $D^{ep}$ is positive semi-definite.

The search direction $d_T^0$ is tangent to the active plastic admissibility constraint; hence, to enforce admissibility for stresses, a step relaxation and stress scaling is performed until $f_j(T) = 0$ for all plastic constraints. The equilibrium condition is preserved by also relaxing and scaling the load factor. The fact that $K$ is positive semi-definite implies that $d_T^0$ is non-negative. The relaxation-scaling stage is based on this remark and reads as follows:

$$
\tilde{T} = p(T + sd_T^0), \quad \tilde{P} = p(P + sd_P^0)
$$

(5.21)

The symbols $\tilde{T}$ and $\tilde{P}$ are new approximations for stress and load factor. The step relaxation factor $s$ is set to 1 at the beginning. The scaling factor $p$ is computed, for each $s$, so that all plastic constraints remain negative and one of them, at least, becomes almost zero. If this value of $p$ renders an approximation for $\tilde{P}$, as given above, lower than $P$ then the relaxation factor is reduced by setting $s \leftarrow \gamma_s^0 s$, where $\gamma_s^0$ is a prescribed parameter; then, $p$ is computed again. This procedure is repeated until $\tilde{P} > P$. The modified direction $(\tilde{T} - T)$ becomes closer to the ascent direction $d_T^0$, each time $s$ is reduced, so that these iterations certainly reach the desired condition.

Equilibrium is exactly enforced at initialization and preserved along the iterative process. To initialize the algorithm, $T = 0$, $P = 0$ and $\lambda_j = -1/f_j(0)$ is used. The algorithm for limit analysis is summarized in Table 5.1. The algorithm requires, besides the gradient, the computation, at each iteration, of the Hessian of the yield function. However, in the hyperbolic case, the Hessian presents singularities and is only positive semi-definite. To address this problem, small perturbation (Eq (5.15)) are introduced based on the characterization of the kernel of the Hessian. They are intended to allow that the matrix $H$ in (5.15) can be inverted as required by (5.19).
I) INITIALISATION
\[ T = 0, \quad P = 0 \]
for each plastic mode
\[ \lambda_j = -1/f_j (0) \]
endfor

II) INCREMENT ESTIMATE

for each element \( i \)
\[ H^{-1} = \left( \sum \lambda_j (\nabla^2 f_j + \epsilon M) \right)^{-1} \]
\[ Q = H^{-1} \nabla f \]
\[ W = \nabla f^T H^{-1} \nabla f - \Lambda^{-1} G \]
\[ D^{ep} = H^{-1} - Q W^{-1} Q^T \]
\[ K' = B^T D^{ep} B \]
Mount \( K' \) in \( K \)
endfor
Solve \( K u = F \)
\[ d_p^0 = \frac{1}{E} \cdot \frac{\gamma}{\gamma} \]
\[ z^0 = d_p^0 \cdot \frac{\gamma}{\gamma} \]
for each element
\[ A^0 = W^{-1} Q^T B z^0 \]
endfor

III) CONVERGENCE CHECK

if \[ ||B z^0 - \Delta \nabla f (T)||_\infty \leq \epsilon_D ||B z^0||_\infty \]
and
for each plastic mode in each element
\[ ||\lambda_j^0|| \leq \epsilon_\lambda \left( \lambda^0 \right)_\infty \]
or
\[ f_j > \epsilon_f f_j (0) \]
then terminate, convergence achieved

IV) STRESS INCREMENT ESTIMATE

for each element \( i \)
\[ d_T^0 = D^{ep} B z^0 \]
endfor

V) STEP RELAXATION AND STRESS SCALING

\[ \gamma_f = \min \left\{ \gamma_j^0, d_p^0 / P \right\} \]
\[ s = 1 \]
repeat until \( \bar{P} > P \)
\[ P^0 = P + s d_p^0 \]
for each element
\[ T^* = T + s d^0 \]
for each plastic mode
Find \( p_j \) such that
\[ f_j (p_j T^*) = \gamma_f f_j (T) \]
endfor
endfor
\[ p = \min p_j \]
\[ \bar{P} = p \cdot P^0 \]
\[ s \leftarrow \gamma_s^0 s \]

VI) UPDATING

\[ P \leftarrow \bar{P} \]
\[ \gamma_\lambda = \min \left\{ \gamma_\lambda^0, \frac{||d_T^0||}{||T||} \right\} \]
for each element
\[ T \leftarrow p T^s \]
for each plastic mode
\[ \lambda_j \leftarrow \max \left( \lambda_j^0, \gamma_\lambda \left( \lambda^0 \right)_\infty \right) \]
endfor
endfor

Table 5.1: Borges' Algorithm for Limit Analysis [adapted from [11], [85]].
5.1.4 Computational Environment

To fully develop the hardness–microstructure relation (5.1), a large number of simulations is required. To achieve this goal, we created a script that interfaces the limit analysis solver just described with an input file that contains the list of parameters, initializes the limit analysis solver and automatically stores the results in a text files.

The structure of the input text file is the following: a first line contains the scheme employed for the resolution (coded by two letters, SC or MT), and the values of all the parameters except the porosity. For future refinement, there is space for up to seven input parameters. The second line specifies the number of different values for the porosity and the third one lists these values. That constitutes a group of three lines. We can add other groups of three lines with different parameters until we mark the end of the file by the symbol "--".

By way of illustration, for a porous material with a Drucker-Prager solid strength criterion \(c_s = 1, \alpha_s = 0.2\), for which we want to investigate six porosities for the self-consistent morphology, the input file reads as:

```
SC 1.000 .200 .000 .000 .000 .000 .000
6
 .001 .050 .150 .250 .350 .450
--
```

5.2 Level I—Results and Validation

We first consider Level I of our model for shales, i.e. the porous clay composite. The hardness-to-cohesion ratio is a function of the semi-apex angle of the conical indenter, \(\theta\), the friction of the pure solid phase, \(\alpha_s\), the packing density \(\eta\), and the percolation threshold \(\eta_0\), introduced to represent two characteristic pore morphologies (see Section 3.3.6): \(\eta_0 = 0\) for the matrix-inclusion morphology captured by the Mori-Tanaka scheme versus \(\eta_0 = 1/2\) for the perfect disordered morphology captured by the self-consistent scheme; hence:

\[
\text{Level I: } \frac{H}{c_s} = \Pi_H (\theta = 70.32^\circ, \alpha_s, \eta, \eta_0)
\] (5.22)
where $\theta = 70.32^\circ$ corresponds to the equivalent cone angle of the Berkovich indenter (Eq. (4.16)). Then, in order to map the values of the hardness-to-cohesion ratio for any parameter of the system (5.22), we vary $\alpha_s \in [0, \sqrt{3}/4]$ according to the limits defined by (3.5); and $\eta \in [\eta_0, 1]$, covering the entire range of the elliptical strength domain, $\eta \in [\eta_0, \eta^{cr}]$, and the hyperbolic strength domain, $\eta \in [\eta^{cr}, 1]$, according to:

$$
\eta - \eta^{cr} (\alpha_s, \eta_0) \begin{cases}
> 0 & \text{Hyperbolic Criterion} \\
= 0 & \text{Limit Parabola} \\
< 0 & \text{Elliptical Criterion}
\end{cases}
$$ (5.23)

where $\eta^{cr} (\alpha_s, \eta_0)$ is the critical packing density expressions (3.61) and (3.62) for the Mori-Tanaka morphology and the self-consistent morphology, respectively.

However, we were unable to achieve convergence with the Limit Analysis Solver for high values of $\alpha_s > 1/\sqrt{3} = 0.57735$. We were not able to identify the reason for this computational limitation. Hence, all results below are for $\alpha_s \in [0, \sqrt{1/3}]$.

5.2.1 Effect of Pore Morphology

Figure 5-1(a-b) display typical simulation results, in form of discrete $H/c_s - \eta$ plots for the Mori-Tanaka morphology (Fig. 5-1(a)) and the self-consistent morphology (Fig. 5-1(b)). For purpose of clarity, we only display the results for four values of $\alpha_s$. There is a clear difference in the way the hardness scales with the packing density between the two pore morphologies: while both morphologies yield a monotone increasing scaling of the hardness with the packing density, the self-consistent scheme is characterized by a vertical asymptote at $\eta = \eta_0 = 1/2$ and a subsequent change in curvature.

The plots in Figure 5-1(a-b) also show the $\eta^{cr} (\alpha_s, \eta_0)$-values, where the criterion changes from an ellipse to an hyperbole. An interesting observation is that the hardness-packing density scaling appears to be continuous over the entire range $\eta \in [\eta_0, 1]$. We will make use of the observation in the later development of fitting functions of the scaling relations.
Figure 5-1: Evolution of the Hardness over cohesion ratio of the porous clay, $H/c_a$, with the packing density, $\eta$, and the solid friction coefficient, $\alpha_s$. (a) using a Mori-Tanaka scheme - (b) using a Self-Consistent scheme.
5.2.2 Comparison with the Elliptical Upper-Bound Solution of Cariou et al.

Hardness–packing density scaling relations of a cohesive-frictional porous composite were first obtained by Cariou et al. in 2006 [19],[20]. The approach pursued by Cariou et al. is based on a computational implementation of the upper-bound theorem of yield design (4.32) for an elliptical strength criterion derived from the effective strain rate approach of Barthelemy and Dormieux (see Eq. (3.66). The restriction to the elliptical case limits the results to packing densities below the critical percolation threshold (5.23), \( \eta_0 \leq \eta < \eta^c (\alpha_s, \eta_0) \). Nevertheless, the range of packing densities for which the homogenized strength criterion is an ellipse provides an excellent means to validate the results we obtain with (i) slightly different expressions of the elliptical parameters (see Section 3.3.7), and (ii) with another limit analysis algorithm. Keeping these two differences in mind, the comparison displayed in Figure 5-2, shows in general an excellent agreement. Furthermore, consistent with the fact that Cariou et al.’s approach provides an upper-bound solution, we observe a slight trend that Cariou’s estimates are just greater than our estimates.

5.2.3 Comparison with Ganneau’s Solution

In order to validate the hardness estimates for the hyperbolic criterion, i.e. for packing densities greater than the critical one, we benchmark our results against published results obtained by Ganneau et al. [45][44], in 2004/05. Ganneau computed upper bound estimates for the hardness of a homogeneous material following a Mohr-Coulomb strength criterion, which he condensed in the form:

\[
\frac{H^+}{C} = \frac{1}{\mu} \sum_{k=1}^{6} (a_k (\theta) \mu)^k
\]  

(5.24)

where \( C \) is the Mohr-Coulomb cohesion and \( \mu = \tan \varphi \) is the Mohr-Coulomb friction coefficient (see Eq. (3.2)); while the \( a_k (\theta) \) -coefficients are fitted to the simulation results. In the case of a Berkovich indenter, \( \theta = 70.32^\circ \), they are: \( a_1 = 5.7946, a_2 = 2.9455, a_3 = -2.6309, a_4 = 4.2903, a_5 = -3.4887, a_6 = 2.7336 \).

Although the Mohr-Coulomb criterion is different from the Drucker-Prager criterion (see Section 3.2.1), it is possible to give bounds for the correspondence between the two, by considering the internal cone and the compression cone, as displayed in Fig. 3-2, and expressed
Figure 5-2: Validation of the elliptical case: Comparison with Cariou’s indentation solutions. (a) Self Consistent scheme, $\alpha_s = 0.0$; (b) Self Consistent scheme, $\alpha_s = 0.2$; (c) Self Consistent scheme, $\alpha_s = 0.4$; (d) Mori Tanaka scheme, $\alpha_s = 0.0$; (e) Mori Tanaka scheme, $\alpha_s = 0.2$; (f) Mori Tanaka scheme, $\alpha_s = 0.4$
Figure 5-3: Validation of the hyperbolic case: Comparison with Ganneau et al.'s solution for a Mohr-Coulomb solid ($\eta = 1$).

by relations (3.6). This provides a means to compare Ganneau's solution with our solutions. Figure 5-3 which displays the scaling of the hardness-to-cohesion ratio with the Mohr-Coulomb friction angle, shows that our estimates are consistent with Ganneau's estimates. Indeed, the trend is similar and Ganneau's values are, as expected, between the internal cone estimate and the compression cone estimate. This is not the case for $\theta = 0$, for which the Mohr-Coulomb criterion becomes a Tresca criterion, and which is beyond the reach of Ganneau's simulation results and fitting function (5.24). Furthermore, we observe that the value obtained with a Mohr-Coulomb criterion is closer to the compression cone than to the internal cone. This is consistent with the fact that indentation activates mostly compressive stress fields.

5.3 Level II–Results: The Effect of Rigid Inclusions

We now turn to the Level II results:

$$\text{Level II: } \frac{H}{c_s} = \Pi_H (\theta, \alpha_s, \eta, \eta_0, f_{inc}, f_0)$$ (5.25)
5.3.1 Morphology Permutations

We remind ourselves that the Level II homogenization step encompasses a priori $2^3 = 8$ different morphological and interface permutations:

- $2 \times$ Level I–pore morphologies: Mori-Tanaka pore morphology ($\eta_0 = 0$) and self-consistent pore morphology ($\eta_0 = 1/2$).

- $2 \times$ Level II–matrix–rigid inclusions morphologies: Mori Tanaka morphology and self-consistent morphology.

- $2 \times$ Level II–interface conditions: perfect adherence and perfect slippery interface.

However, for hardness analysis we restrict ourselves to the case of perfect adherence, which reduces the eight cases to the following four combinations:

<table>
<thead>
<tr>
<th>Level I Pore Morphology</th>
<th>Level II Morphology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Self Consistent</td>
<td>Self Consistent</td>
</tr>
<tr>
<td>Mori Tanaka</td>
<td>Mori Tanaka</td>
</tr>
</tbody>
</table>

SC - SC                 SC - MT
MT - SC                 MT - MT

5.3.2 The Effects of Rigid Inclusions

The results of the four combinations, for a reasonable friction coefficient $\alpha = 0.12$, are displayed in Figures 5-4 and 5-5, in form of parameter plots that show the effect of the inclusion volume fraction $f_{inc}$ on the hardness-to-cohesion ratio. The following two observations deserve attention:

1. The effect of rigid inclusions on the hardness-to-cohesion ratio depends on the Level I packing $\eta$: The higher the Level I packing $\eta$, the more pronounced the $H/c_s$ enhancement with increasing Level II inclusion fraction $f_{inc}$. Vice versa, the effect of rigid inclusions at level II for low packed Level I systems is truly negligible. This observation holds for all four combinations.

2. The effect of rigid inclusions on the hardness-to-cohesion ratio depends on the Level II morphology: The $H/c_s$ enhancement is more pronounced in the case of a perfectly

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disordered Level II morphology (MT-SC and SC-SC, shown in the (b)-figures in Figs. 5-4 and 5-5), than in the case of a Level II matrix-inclusion morphology (MT-MT and SC-MT, shown in the (a)-figures in Figs. 5-4 and 5-5). This observation holds irrespective of the Level I pore morphology.

In summary, the more packed the solid at level I, and the more disordered the matrix-inclusion composite, the greater the effect of rigid inclusions on the hardness-to-cohesion ratio.

5.4 Summary of Results: Scaling Relations

The aim of this Section is to derive fitting functions that summarize the discrete simulation results in closed form expressions so that these expressions can be used for data analysis. It should be emphasized that the expressions derived below are valid provided the following conditions:

1. Berkovich indenter ($\theta = 70.32^\circ$).

2. Solid friction coefficient, $\alpha_s \in [0, \sqrt{1/3}]$. As the behavior of the hardness becomes very steep for high friction values, the formulas derived below are accurate only for $\alpha_s \in [0, 0.5]$.

3. Perfect adherence of inclusions with porous matrix.

The fitting functions encompass both the elliptical case and the hyperbolic case. A complete listing of the discrete values of $H/c^s$ for Level I and Level II is given in the Appendix.

5.4.1 Level I: Cohesive-Frictional Porous Composite

Following a data analysis, the format of the scaling relations at Level I is chosen in the following form:

$$H = h_s(c_s, \alpha_s) \times \Pi_H^1(\alpha_s, \eta, \eta_0)$$

(5.26)

where $h_s = h_s(c_s, \alpha_s) = \lim_{\eta \to 1} H$ is the asymptotic hardness of a cohesive-frictional solid phase that obeys to the Drucker-Prager criterion (see Section 5.2.3). This asymptotic value does not depend on the employed linear homogenization scheme, but relates only to the solid's
Figure 5-4: Evolution of the Hardness over cohesion ratio of the Level II composite, $H/c_s$, with the packing density, $\eta$, and the inclusion volume fraction, $f_{inc}$. Results obtained for a solid friction coefficient, $\alpha_s = 0.12$, and with perfect adhesion. (a) using a Mori-Tanaka scheme - (b) using a Self-Consistent scheme.
Figure 5-5: Evolution of the Hardness over cohesion ratio of the Level II composite, $H/c_s$, with the packing density, $\eta$, and the inclusion volume fraction, $f_{inc}$. Results obtained for a solid friction coefficient, $\alpha_s = 0.12$, and with imperfect interfaces. (a) using a Mori-Tanaka scheme - (b) using a Self-Consistent scheme.
cohesion c_s and friction coefficient \(\alpha_s\):

\[
h_s = c_s \times A \left(1 + B\alpha_s + (C\alpha_s)^3 + (D\alpha_s)^{10}\right)
\]

(5.27)

with:

\[
\begin{align*}
A &= 4.76438 \\
B &= 2.5934 \\
C &= 2.1860 \\
D &= 1.6777
\end{align*}
\]

In return, the dimensionless function \(\Pi_H^{I}\) depends on the packing density \(\eta\), the homogenization scheme, represented by the solid’s percolation threshold \(\eta_0\), as well as on the solid’s friction coefficient \(\alpha_s\). For a given percolation threshold (i.e. Level I–homogenization scheme), we choose:

\[
\Pi_H^{I}(\alpha_s, \eta, \eta_0) = \Pi_1(\eta, \eta_0) + \alpha_s (1 - \eta) \Pi_2(\alpha_s, \eta, \eta_0)
\]

(5.28)

where \(\Pi_1(\eta, \eta_0) = \Pi_H^{I}(\alpha_s = 0, \eta, \eta_0) \in [0, 1]\) is the frictionless portion of the function. The dimensionless functions \(\Pi_1(\eta, \eta_0)\) and \(\Pi_2(\alpha_s, \eta, \eta_0)\) are fitted for the two considered pore morphologies: Mori–Tanaka scheme \((\eta_0 = 0)\) and self-consistent scheme \((\eta_0 = 1/2)\).

**Level I: Mori–Tanaka Scheme: \(\eta_0 = 0\)**

For the Mori Tanaka scheme, which corresponds to a matrix-pore morphology, we obtain the following expressions for \(\Pi_1(\eta, \eta_0 = 0) = \Pi_1^{mt}(\eta)\) and \(\Pi_2(\alpha_s, \eta, \eta_0 = 0) = \Pi_2^{mt}(\alpha_s, \eta)\):

\[
\begin{align*}
\Pi_1^{mt}(\eta) &= \eta \left(1 + a (1 - \eta) + b (1 - \eta)^2 + c (1 - \eta)^3\right) \\
\Pi_2^{mt}(\alpha_s, \eta) &= \alpha_s \eta^2 (d + e (1 - \eta) + f (1 - \eta) \alpha_s + g \alpha_s^2)
\end{align*}
\]

(5.29)
Level I: Self-Consistent Scheme: $\eta_0 = 1/2$

For the self-consistent scheme, which corresponds to a perfectly disorder porous material, we obtain the following expressions for $\Pi_1 (\eta)$ and $\Pi_2 (\alpha, \eta)$:

$$\Pi_1 (\eta) = \frac{\sqrt{2(2\eta - 1) - (2\eta - 1)}}{\sqrt{2} - 1} \left( 1 + a(1 - \eta) + b(1 - \eta)^2 + c(1 - \eta)^3 \right)$$

$$\Pi_2 (\alpha, \eta) = \frac{2\eta - 1}{2} \left( d + e(1 - \eta) + f(1 - \eta) \alpha_s + g\alpha_s^3 \right)$$

with

$$MT: \begin{cases} a = -1.2078 & d = 8.7145 \\ b = 0.4907 & e = -40.6615 \\ c = -1.7257 & f = 74.0617 \\ & g = -64.094 \end{cases}$$

$$SC: \begin{cases} a = -5.3678 & d = 6.7374 \\ b = 12.1933 & e = -39.5893 \\ c = -10.3071 & f = 34.3216 \\ & g = -21.2053 \end{cases}$$

5.4.2 Level II: Porous Matrix–Rigid Inclusion Composite

The introduction of rigid inclusions at Level II enhances the value of the hardness (see Section 5.3.2). In order to be consistent with the scaling relations reported for Level I, we employ the following format for the Level II scaling relations:

$$H = h_s (c_s, \alpha_s) \times \Pi_1^I (\alpha_s, \eta, \eta_0) \times \Pi_2^I (\alpha_s, \eta, \eta_0, f_{inc}, f_0)$$

(5.31)

where $h_s (c_s, \alpha_s)$ is given by (5.27), and $\Pi_2^I (\alpha_s, \eta, \eta_0)$ by (5.28).

The dimensionless function $\Pi_2^I$ thus expresses the hardness enhancement introduced by the addition of rigid inclusions, and is expressed as follow:

$$\Pi_2^I (\alpha_s, \eta, \eta_0, f_{inc}, f_0) = 1 + \Pi_3 (\alpha_s, f_{inc}, f_0) \times \Pi_4 (\alpha_s, \eta, \eta_0, f_{inc}, f_0)$$

(5.32)
where \( \Pi_4 = 1 \) for \( \eta = 1 \), meaning that \( 1 + \Pi_3 \) is the correction factor of the top point (solid phase + inclusions; no pores). This point does not depend on the Level I homogenization scheme since there are no pores. In other words, \( \Pi_3 \) only depends on the Level II homogenization scheme (represented by \( f_0 \)), while \( \Pi_4 \) depends on both \( (\eta_0, f_0) \).

### Self-Consistent + Self-Consistent

\[
\Pi_3 (\alpha_s, f_{inc}) = f_{inc} (h + if_{inc} + j f_{inc}^3 + k\alpha_s + t\alpha_s f_{inc}^4 + m\alpha_s^4 f_{inc}^4) \tag{5.33}
\]

\[
\Pi_4 (\alpha_s, f_{inc}, \eta) = (2\eta - 1)^2 \left[ 1 + (1 - \eta)^2 \left(n f_{inc}^2 + o f_{inc}^2 (1 - \eta)^2 + p\alpha_s f_{inc}^2 + q\alpha_s f_{inc}^2 (1 - \eta) \right) \right] \tag{5.34}
\]

with

\[
\begin{align*}
SC - SC: & \\
& \begin{cases} 
    h = 0.7983 \\
    i = 1.0205 \\
    j = 40.498 \\
    k = 2.20486 \\
    l = 654.518 \\
    m = 1485.08 \\
n = -92.0907 \\
o = 1341.11 \\
p = 452.261 \\
q = -2022.59 
\end{cases}
\end{align*}
\]

### Self-Consistent + Mori-Tanaka

\[
\Pi_3 (\alpha_s, f_{inc}) = f_{inc} (h + if_{inc} + j f_{inc}^3 + k\alpha_s + t\alpha_s f_{inc}^4 + m\alpha_s^4 f_{inc}^4) \tag{5.35}
\]

\[
\Pi_4 (\alpha_s, f_{inc}, \eta) = (2\eta - 1)^2 \left[ 1 + (1 - \eta)^2 (n + o) f_{inc} + p\alpha_s (1 - \eta) + q\alpha_s (1 - \eta)^2 \right] \tag{5.36}
\]

with

\[
\begin{align*}
SC - MT: & \\
& \begin{cases} 
    h = 0.7327 \\
    i = -0.5891 \\
    j = 26.2921 \\
    k = -106.032 \\
    l = 131.301 \\
    m = 80.9915 \\
n = -174.794 \\
o = 674.91 \\
p = 177.007 \\
q = -723.504 
\end{cases}
\end{align*}
\]

### Mori-Tanaka + Self-Consistent

\[
\Pi_3 (\alpha_s, f_{inc}) = f_{inc} (h + if_{inc} + j f_{inc}^3 + k\alpha_s + t\alpha_s f_{inc}^4 + m\alpha_s^4 f_{inc}^4) \tag{5.37}
\]

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\[ \Pi_4(\alpha_s, f_{inc}, \eta) = \eta^2 \left[ 1 + (1 - \eta) \left( n f_{inc} + o f_{inc} (1 - \eta)^2 + p \alpha_s f_{inc} + q \alpha_s f_{inc} (1 - \eta) \right) \right] \] (5.38)

\[
\begin{align*}
&h = 0.7983 \\
i = 1.0205 \\
j = 40.498 \\
k = 2.20486 \\
l = 654.518 \\
m = 1485.08
\end{align*}
\]

MT - SC:

\[
\begin{align*}
h &= 0.7983 \\
i &= 1.0205 \\
j &= 40.498 \\
k &= 2.20486 \\
l &= 654.518 \\
m &= 1485.08
\end{align*}
\]

Mori-Tanaka + Mori-Tanaka

\[ \Pi_3(\alpha_s, f_{inc}) = f_{inc} (h + if_{inc}^2 + j\alpha_s^2 + k\alpha_s^3 + l\alpha_s^4 + m\alpha_s^4 f_{inc}) \] (5.39)

\[ \Pi_4(\alpha_s, f_{inc}, \eta) = \eta^2 \left[ 1 + (1 - \eta) \left( n (1 - \eta) + o (1 - \eta)^2 + p \alpha_s (1 - \eta) + q \alpha_s (1 - \eta)^2 \right) \right] \] (5.40)

with

\[
\begin{align*}
h &= 0.7327 \\
i &= -0.5891 \\
j &= 26.2921 \\
k &= -106.032 \\
l &= 131.301 \\
m &= 80.9915
\end{align*}
\]

MT - MT:

\[
\begin{align*}
h &= 0.7327 \\
i &= -0.5891 \\
j &= 26.2921 \\
k &= -106.032 \\
l &= 131.301 \\
m &= 80.9915
\end{align*}
\]

5.5 Chapter Summary

The ultimate goal of indentation analysis of heterogeneous materials is the reverse analysis of microstructural parameters \((\eta, f_{inc})\) and constituent material properties \((c_s, \alpha_s)\) of the indented material. The contribution of this Chapter is the implementation of the multi-scale strength homogenization model developed in Chapter 3 in form of hardness–microstructure relations. To this end, we employed a limit analysis solver that is sufficiently flexible to solve for the hardness-to-cohesion ratio for any second order strength criterion, which includes the elliptical and hyperbolic case. While the elliptical case has been investigated before \([19],[20]\), it is, to our knowledge, the first time that the solution of the hyperbolic case is achieved. Moreover, the solution of the elliptical case with the technique developed by Borges requires approximately 30
seconds compared to more than an hour required with the upper bound optimization algorithm developed by Cariou [19]. We thus extended the domain of application of the hardness-packing density scaling relations of cohesive-frictional porous materials to the hyperbolic case. In turn, this extension now provides hardness-packing scaling relations over the entire range of solid packing densities, from the percolation threshold to the pure solid state. Furthermore, the addition of rigid inclusions (with perfect adherence) is found to enhance the hardness of the cohesive-frictional porous material; and this the more the higher packed the porous material (at Level I) and the more disordered the porous matrix-rigid inclusion composite at Level II. Finally, by synthesizing the discrete simulation results into closed-form expressions, the hardness-microstructure relations are ready to be employed for day-to-day indentation analysis of the hardness of porous materials. These data will be used in the next (and last part) of this report for the indentation analysis of microstructure and properties of the porous clay phase in shale.
Part IV

Application in Nanoindentation

Analysis of Shale
Chapter 6

Algorithm for the Reverse Analysis of Shale Microstructure

This part employs the hardness-packing density scaling relations in nanoindentation analysis of shale. To this end, this Chapter develops an original algorithm for the reverse analysis of the packing density and particle properties from nanoindentation data: indentation modulus, $M$, and indentation hardness, $H$. The fundamental idea of the algorithm is that $M$ and $H$ sense the same microstructure, and that $N$ indentation tests which provide $2N$ data points $(M, H)_i, i = 1, N$, can be used in a reverse application of the scaling relations to determine $N$ packing densities $(\eta_i, i = 1, N)$ and $n \leq N$ solid properties [102]. This Chapter translates this idea into a robust computational algorithm for shale. The next chapter applies this algorithm to a large range of shale materials of different geographical origins, mineralogy, density, porosity, etc.

6.1 Sensing Microstructure from Indentation

6.1.1 $(M, H)$ Scaling Relations of the Porous Composite

To motivate the forthcoming algorithmic developments, consider a large array of $N$ indentation tests (indentation grid) on a surface of a cohesive-frictional porous material half-space. The distance between indents (grid spacing) is sufficiently large so to exclude any interaction between
The packing density \( \eta_i \) may vary from grid-point to grid-point, but the solid phase is assumed to be the same. Assuming scale separability, the indentation modulus \( M_i \) and the indentation hardness \( H_i \), which are extracted from the indentation test at each grid-point, are composite properties, representative of the homogenized response of the porous material; that is [102]:

\[
M_i = m_s \times \Pi_M \left( \frac{C_{ijkl}^s}{m_s}, \eta_i, \eta_0 \right) \tag{6.1a}
\]

\[
H_i = h_s (c_s, \alpha_s) \times \Pi_H (\alpha_s, \eta_i, \eta_0) \tag{6.1b}
\]

where \( (m_s, h_s) = \lim_{\eta \to 1} (M, H) \), \( C_{ijkl}^s \) and \( \alpha_s \) are solid properties, while \( \eta_i \) stands for the local solid packing density. In a forward application, use of the scaling relations (6.1a) and (6.1b), requires knowledge of \( n \) solid properties \( (m_s, C_{ijkl}^s, c_s, \alpha_s) \) and of the solid’s packing density \( \eta_i \) to determine the composite indentation quantities \( M_i \) and \( H_i \). In a reverse application, \( N \geq n \) indentation tests are required, to determine from experimental \( (M, H) \) values the solid properties \( (m_s, C_{ijkl}^s, c_s, \alpha_s) \) and the solid’s packing density \( \eta_i \). Therefore, provided the existence of a unique solid phase present in the porous microstructure, the scaling relations are a versatile tool to probe the microstructure sensed by the large array of grid indentation tests.

The input to such a reverse analysis is a data set composed of \( N \) sets of \( (M, H) \) values. A typical data set for shale is presented in Figure 6-1, in form of a \( M - H \) plot. While there is some spread in data, we can clearly identify a region of high concentration of \( (M, H) \) points. These points are also observed in the histograms of the distribution of \( M \) and \( H \) displayed in Figure 6-2. In fact, for shales, these points represent indents into the porous clay phase, while the large spread of data at higher stiffness and hardness represent indents either into inclusions or close to an inclusion, such that the indentation response is disrupted and is actually a composite response.

The algorithm will focus on the porous clay phase only, which is assumed to be composed of a single solid phase and porosity which varies locally within the microstructure. Although there may be a certain variability in the mechanical properties of the solid phase, the scale separability condition together with the central limit theorem produces characteristic quantities
Figure 6-1: Typical nanoindentation data set of shale [courtesy of C. Bobko, MIT; data from Shale #1 of GeoGenome data base].

that are constant from one indent to another\(^1\), provided that:

\[ N \gg n \] \hspace{1cm} (6.2)

### 6.1.2 Shale Model Assumptions

The application of (6.1a) and (6.1b) to shale requires to choose an appropriate micromechanical representation of the porous clay phase. Recent nanomechanical results reported by Ulm and Abousleiman [101] and Bobko and Ulm [10] establish a unique nanogranular mechanical signature of shales porous clay phase (Level I):

- **Percolation Threshold**: The elastic behavior of the porous clay phase in shales is characterized by a clay-packing density percolation threshold of \( \eta_0 = 0.5 \), below which the material has no appreciable stiffness (nor strength).

\(^1\)Indeed, we can consider the mechanical properties of the clay particles as independent and identically distributed random variables. Then, as the number of particles below the indenter is large (scale separability condition), the central limit theorem leads to a narrow distribution around a characteristic quantity constant from one indent to another.
Figure 6-2: Statistical analysis of a \((M, H)\) data set of shale showing one dominating phase that represents the porous clay phase.

- Scaling of Elastic Anisotropy: Above the percolation threshold, the elastic anisotropy of the porous clay phase in shales scales with the clay packing density almost linearly toward a unique set of asymptotic clay particle stiffness values, which are insensitive to the particular clay mineralogy.

- Isotropic Hardness Behavior: Above the percolation threshold, there is no appreciable difference in hardness values between different directions, meaning that strength behavior of the porous clay phase can be assumed as isotropic.

By way of illustration, Figure 6-3 displays the scaling of the elasticity content of the porous clay phase as a function of the clay packing density \(\eta\) for seven shale materials of different origin and mineralogy. The elasticity content was obtained by subtracting from the macroscopic transversely isotropic elasticity constants (level II) the effect of the silt inclusion by means of a Reuss bound. The elasticity constants so obtained are condensed into the equivalent indentation moduli (4.6) and (4.7), and plotted against the clay packing density. The results illustrate that the elementary building block of shale is intrinsically anisotropic as far as the elasticity is concerned, and that the anisotropy increases as clay packing density increases; and they suggest the following simplified elastic scaling relation (6.1a):

\[
M_i (g_j) = m_s^i \times \begin{cases} 
0 & \eta < \eta_0 = 1/2 \\
(2\eta - 1) & \eta \geq \eta_0 = 1/2
\end{cases}
\]  

(6.3)
Figure 6-3: Porous clay stiffness (condensed into indentation moduli)–clay packing density scaling backcalculated from UPV elasticity measurements of various shale materials [from [77]].

where $\varepsilon_j$ ($j = 1, 3$) stands for the indentation directions ($\varepsilon_1$ = normal to the axis of the material symmetry, $\varepsilon_3$ = normal-to-bedding direction), and $m^j_k = \lim_{\eta \to 1} M(\varepsilon_j)$; ($j = 1, 3$) are the particle-to-particle contact stiffness values:

\[
\begin{align*}
    m^1_s &= 26 \text{ GPa} \\
    m^3_s &= 17 \text{ GPa}
\end{align*}
\]

In contrast to the strength properties, the particle elasticity properties are well established by now [77]. This is why we concentrate our effort on the determination of the strength properties of the solid clay phase, using the hardness-packing density scaling relations for the disordered cohesive-frictional solid developed in Chapter 5. The unknown of the reverse analysis, therefore, are the cohesion, $c_s$, the friction coefficient, $\alpha_s$ and the packing densities $\eta_i$. In return, the values
of \( m^j \) will be fixed "close" to the values reported in Eqs. (6.4) and (6.5). How "close" and what "close" means, will be specified in the sequel.

### 6.2 Reverse Algorithm

This Section provides details of the algorithm for the reverse analysis of the strength parameters and packing densities from \((M, H)\) indentation data.

#### 6.2.1 Indentation Data Filtering

The first step in the algorithm is the determination of the \((M, H)\) data set that represent the porous clay phase in shale nanoindentation. This set is associated with the first Gaussian pic in the histograms 6-2, and is a subset of the total number of tests. It is selected according to the following criteria:

1. \( M_i \)-values representing the porous clay phase must be smaller than the asymptotic values \( m^j_s \) given by (6.4) and (6.5). A cut value is introduced as a percentage of the solid modulus:

   \[
   \frac{M_i}{m^j_s} \leq X_{cut}
   \]  

2. This cut value is compared with a visual inspection of the histogram of \( M_i \) which allows us to identify the porous clay phase as a statistical phase, see Figure 6-4, and separate it from \( M_i \) values representing composite responses.

3. Finally, in order to get rid of irrelevant points that were not eliminated by the cut and that would distort subsequent analysis, we filter the data set by eliminating all points that are clearly off the main trend. These points are usually due to the presence of rigid inclusions close to the indented region (composite response). To do so, we look for the points that are always among the \( x\% \) worst points of the data set for any \( \alpha_s \) (typically, \( x \) may be taken equal to 5). A typical result is sketched in Fig. 6-5.
Figure 6-4: Principle of determination of the cut on the indentation modulus (Shale #1)

Figure 6-5: Example of data filtering
6.2.2 Error Minimization

The second step in the reverse analysis consists of minimizing the error between the experimental data \((M, H)\), and the model response (6.1). The general idea is to compute the total error (or "cost function") and keep the set of parameters that will minimize this total error. For a given set of parameters \(\{\eta, m_s, c_s, \alpha_s\}\), the error created by a point of the data set is due to the difference between the value of the predicted modulus \(M_{th}(\eta, m_s)\) and hardness \(H_{th}(\eta, c_s, \alpha_s)\) (r.h.s. of Eqs. (6.1)) and the experimental values \(M_{exp}\) and \(H_{exp}\). We studied the influence of the three different definitions of the error:

- **Absolute Error**: The absolute error is defined by

\[
S = (M_{exp} - M_{th}(\eta, m_s))^2 + (H_{exp} - H_{th}(\eta, c_s, \alpha_s))^2
\]  

(6.7)

The problem with this error is that it will give more importance to points with high values compared to points with lower values. Since in general the indentation modulus is much larger than the hardness (if expressed in the same unit), the absolute error will lead to a fit of only \(M\) and not of \(H\).

- **Relative Error**: The relative error is defined by:

\[
S = \left(\frac{M_{exp} - M_{th}(\eta, m_s)}{M_{exp}}\right)^2 + \left(\frac{H_{exp} - H_{th}(\eta, c_s, \alpha_s)}{H_{exp}}\right)^2
\]  

(6.8)

It has the advantage that it does not favor high values of \(M\) and \(H\). However, it will give somewhat more importance to points with low values of \(M\) and \(H\) because of the division by small values of \(M_{exp}\) and \(H_{exp}\). The result will be a "cone-like" fitting where the relative error will be quite constant for all packing densities.

- **Normalized Absolute Error**: The "normalized absolute error" uses the same normalization factors, \(M_0\) and \(H_0\) (typically close to \(m_s\) and \(h_s\)), for the entire data set:

\[
S = \left(\frac{M_{exp} - M_{th}(\eta, m_s)}{M_0}\right)^2 + \left(\frac{H_{exp} - H_{th}(\eta, c_s, \alpha_s)}{H_0}\right)^2
\]  

(6.9)
Then the resulting fit does not favor the modulus over the hardness, and it leads to a "strip-like" fitting, which makes more physical sense than the relative error. This is the error we use in our algorithm.

The parameters that lead to the best fit are the solution of the following minimization problem:

$$\min_{\text{Vect}_{\eta}, m_s, c_s, \alpha_s} \sum_i S_i (\eta_i, m_s, c_s, \alpha_s)$$  \hspace{1cm} (6.10)

where $\text{Vect}_{\eta}$ is the vector of all the packings of all indents: $\text{Vect}_{\eta} = [\eta_1, ..., \eta_N]$. Because of the independence of each $\eta_i$, the minimization problem can be rewritten as:

$$\min_{m_s, c_s, \alpha_s} \sum_i \left[ \min_{\eta_i} S_i (\eta_i, m_s, c_s, \alpha_s) \right]$$  \hspace{1cm} (6.11)

Therefore, for a given set $\{m_s, c_s, \alpha_s\}$, we look for the optimal packing density for each point, $\min_{\eta_i} S_i (\eta_i, m_s, c_s, \alpha_s)$, and then compute the total error, $\sum_i \left[ \min_{\eta_i} S_i (\eta_i, m_s, c_s, \alpha_s) \right]$. Because the function $S_i (\eta_i, m_s, c_s, \alpha_s)$ is not always convex, we will use a minimization procedure based on testing rather than on a gradient algorithm.

In order to have an idea of how the error relates to the choice of effective quantities, we developed a rough statistical model. We consider that there is a certain intrinsic variability in the solid properties such that the solid indentation modulus $m_s$ varies around a given value $m_s^0$, the cohesion varies around $c_s^0$ and the friction coefficient around $\alpha_s^0$ (Fig. 6-6).
Figure 6-7: Distance to the model curve in the $(M, H)$ plane, $d_{\text{exp}}-th^0$.

The parametric plot $M(\eta, m_s^0, H(\eta, c_s^0, \alpha_s^0))$ defines the best fitting curve to the experimental $M - H$ data. Because of the great number of indents, we assume that the distance to this best fitting curve in the normalized plan follows a normal distribution (Fig. 6-7):

$$d_{\text{exp}}-th^0 \sim \mathcal{N}(0; \sigma^2)$$ (6.12)

It is important to note that the square of this distance is equal to the normalized absolute error $\min_S \left( \frac{1}{n_i} \sum (\eta_i, m_s^0, c_s^0, \alpha_s^0) \right)$. Now, let us consider a different fitting $M - H$ curve based on non-optimal values of $m_s, c_s$ and $\alpha_s$. The expectation of the square of the distance to this curve is:

$$\langle d_{\text{exp}}^2-th^0 \rangle = \left\langle \left[ d_{\text{exp}}-th^0 + (d_{\text{exp}}-th - d_{\text{exp}}-th^0) \right]^2 \right\rangle$$ (6.13)

If we fix the packing density and observe the value of the second term for a large number of experimental points, we find that the difference $d_{\text{exp}}-th - d_{\text{exp}}-th^0$ is actually equal to the distance between the two curves at this packing density, $d_{th-th^0}$, and it is constant. So by taking it out of the brackets and since the expectation of $d_{\text{exp}}-th^0$ has been assumed to be zero, we
conclude that the second term tends to zero. So we are left with:

\[
\langle d_{\text{exp} - th}^2 \rangle = \langle d_{\text{exp} - th_0}^2 \rangle + \langle (d_{\text{exp} - th} - d_{\text{exp} - th_0})^2 \rangle
\]  

(6.14)

Expressed in term of the error \(S_i\) this relation becomes:

\[
\frac{1}{N} \sum_{i=1}^{N} \left[ \min_{\eta_i} S_i(\eta_i, m_s, c_s, \alpha_s) \right] = \frac{1}{N} \sum_{i=1}^{N} \left[ \min_{\eta_i} S_i(\eta_i, m_s^0, c_s^0, \alpha_s^0) \right] + \langle (d_{\text{exp} - th} - d_{\text{exp} - th_0})^2 \rangle
\]  

(6.15)

The rightmost term quantifies the distance to the best fitting curve in the normalized plan. The minimum is achieved for the effective parameters \(\{m_s^0, c_s^0, \alpha_s^0\}\); so that:

\[
\frac{1}{N} \sum_{i=1}^{N} \left[ \min_{\eta_i} S_i(\eta_i, m_s, c_s, \alpha_s) \right] = \min_{m_s, c_s, \alpha_s} \left[ \frac{1}{N} \sum_{i=1}^{N} \left[ \min_{\eta_i} S_i(\eta_i, m_s^0, c_s^0, \alpha_s^0) \right] \right] + \bar{d}_{th-th_0}^2
\]  

(6.16)

where \(\bar{d}_{th-th_0}^2\) given by,

\[
\bar{d}_{th-th_0}^2 = \langle (d_{\text{exp} - th} - d_{\text{exp} - th_0})^2 \rangle
\]  

(6.17)

quantifies the inaccuracy of the fitting curve.

### 6.2.3 Statistical Determination of Friction

The search of the optimal set of parameters \(\{m_s^0, c_s^0, \alpha_s^0\}\) from the minimization of the total error (Eq. 6.11) faces numerical problems and does not give reproducible accurate estimates. This is the reason why we fix the value of the solid indentation modulus \(m_s\) to known values (6.4) and (6.5), and focus on the determination of the strength parameters \(c_s\) and \(\alpha_s\) and of the packing density distribution. However, we will also consider values of \(m_s \pm 10\%\) away from these estimates. As the isolation of the porous phase data is also a critical point, we will determine a reference cut and deviate \(\pm 5\%\) away from it. Therefore we will have \(3 \times 3 = 9\) possible combinations for the values of the cut and the modulus.

This statistical approach aims at allowing a certain flexibility in the choice of the cut and of \(m_s\), and to see how the corresponding estimates of \(\alpha_s\) overlap and lead to a central estimate of \(\alpha_s\). For each combination, we store the "good values" of \(\alpha_s\) in a result vector. Consistently
with the previous model, a "good solution" is defined by:

\[
\min_{\alpha_s} \left( \frac{1}{N} \sum_{i=1}^{N} \left[ \min_{\eta_i} S_i (\eta_i, m_s, c_s, \alpha_s) \right] \right) - \min_{\alpha_s} \frac{1}{N} \sum_{i=1}^{N} \left[ \min_{\eta_i} S_i (\eta_i, m_s, c_s, \alpha_s) \right] \leq \varepsilon
\]  

(6.18)

where we typically chose \( \varepsilon = 0.005 \).

In most cases, the values of \( \alpha_s \) stored in the result vector turn out to be centered around a peak value as shown in Figure 7-6. Similarly to Figure 6-6, this value may be considered as the central one and is the one we will report. As a result, this technique provides us with a stable estimation of \( \alpha_s \) since it does not rely just on one fit but on nine. This procedure provides us with a means to evaluate the sensitivity of the value of \( \alpha_s \) so obtained, which is also reported (as error bars).
6.2.4 Determination of Packing Density and Cohesion

In order to complete our analysis of the nanomechanical properties of the porous phase, we want to report the value of the solid cohesion, \( c_s \), as well as the distribution of the packing densities, \( \text{Vect}_\eta \). The algorithm provides a value of the friction coefficient, which does not radically depend on the choice of the cut and \( m_s \), since the statistical approach smooths this influence. On the other hand, the dependence of \( c_s \) and \( \text{Vect}_\eta \) on the choice \( m_s \) turns out to be quite significant. However, as this is a bulk property it is quite constant from sample to sample and the possible variability is reduced. So we decide to fix the cut and \( m_s \) to their central values and determine \( c_s \) and \( \text{Vect}_\eta \) based on the value of \( \alpha_s \) previously obtained.

### 6.3 Chapter Summary

The algorithm presented in this Chapter aims at a reverse analysis of the microstructure of cohesive-frictional porous materials based on the nanocontact response. It translates the theoretical-computational developments presented in previous chapters into an efficient tool for the day-to-day indentation practice. The sole input to the algorithm are measured indentation moduli \( M \), and hardness \( H \), and the solid stiffness \( m_s \). The output are particle strength properties \((c_s, \alpha_s)\) and packing density distributions \( \text{Vect}_\eta \). This algorithm will be put to work in the next chapter for the reverse analysis of microstructure and constituent properties of the porous clay phase in shales.
Chapter 7

Application to Shale

This chapter presents a first application of the tools developed throughout this thesis to shales at different scales (Fig. 3-1):

- At Level I of the porous clay phase, we make use of the hardness-packing density scaling relations developed in Chapter 5 in the reverse algorithm developed in Chapter 6 to analyze packing density distributions and constituents strength properties of the elementary building block of shales from nanoindentation results of shales. Eleven different shale materials are investigated, for which the nanoindentation results were obtained by Chris Bobko as part of his Ph.D. work at MIT.

- At Level II of the porous clay-silt inclusion composite, we make use of the homogenization results developed in Chapter 3 to predict how the cohesive-frictional nature of the elementary building block potentially affects the macroscopic strength domain of shales in the presence of silt inclusions with and without adherence.

7.1 Clay Packing Density Analysis

This and the next section presents the results of a fruitful collaboration with Chris Bobko, Ph.D. student at MIT.
7.1.1 Materials

Eleven different shale materials, obtained from core samples, were tested in this study. These materials are part of the GeoGenome project administered through the GeoGenome Industry Consortium. Six out of eleven materials are the GeoGenome benchmark shales [10], the remaining five are Woodford shales [2]. Information regarding the porosity, bulk density, and mineralogy (in terms of a ratio of non-clay inclusion to solid volume fraction) was provided with the samples. The tested shales have a relatively wide range of mineralogies and porosities, confirming the known diversity of shale materials.

Clay packing density is easy to calculate from mineralogy, bulk density and porosity. The total volume is partitioned into three categories, porosity, \( \phi \), clay volume fraction, \( f_c \), and non-clay inclusion volume, \( f_{inc} \), that sum to one. This information permits the calculation of the clay packing density, \( \eta \), given by:

\[
\eta = \frac{f_c}{1 - f_{inc}} = 1 - \frac{\phi}{1 - f_{inc}} \tag{7.1}
\]

The clay packing density may vary depending on how the porosity is measured. It is well documented that mercury intrusion porosimetry underestimates the actual porosity [35], while estimation of porosity by using the bulk density and mineralogy information gives a higher value of porosity. This leads to a variation in the calculation of \( f_{inc} \) and \( \eta \) as values calculated from porosity are smaller than those calculated from the bulk density.

7.1.2 Indentation Test Parameters

The nanoindentation test campaigns on all 11 shales was performed by Chris Bobko [10]. The material samples (small core sections) were stored in conditions near to the natural relative humidity of the materials, either in desiccators with salt solutions or in tightly sealed vessels filled with decane. Samples were cut to expose surfaces parallel and perpendicular to the isotropy planes of the material.

As previously discussed, the analysis of nanoindentation assumes that indentation occurs on an infinitely flat surface. Although this is not possible in practice, a surface preparation program was developed which minimizes both the roughness and sample disturbance of the material [70].
Figure 7-1: 3-d representation of AFM data, after an indent. The indent is clearly deeper than scale of the roughness, and is large enough to feel the response of a porous composite of clay particles. [Courtesy of C. Bobko [10]].

The samples are first mounted to stainless steel plates for mounting in the indenter. They are then ground by hand on 45 grit diamond paper (with the help of a jig) to make the surface flat and parallel with the mounting plate. The samples were then polished with a 1 micron diamond paste (oil-based) on TexMet pads (Buehler) mounted to a lapping wheel. From AFM testing, the RMS roughness obtained with this polishing procedure measurements was found to be on the order of 150 to 300 nm (Fig. 7-1).

Force driven nanoindentation tests operated to a maximum force of $P = 4.8$ mN were carried out on all samples, leading to an average maximum indentation depth on the order of $h_{\text{max}} = 500 - 2,000$ nm depending on the packing density of the porous clay phase, which satisfies on average the scale separability condition (4.24) required for the indentation analysis of $(M, H)$ based on continuum models.
Shale samples were tested in the (macroscopically identified) direction of symmetry ($\varepsilon_3$) and normal to the direction of symmetry ($\varepsilon_1$). For each exposed surface, typically $N = 300$ tests were carried out on a regular grid of $l = 30$ $\mu$m grid spacing (distance between indents), which yields a sufficient large number of tests over a wide area to achieve statistical independence and good sampling representation.

### 7.1.3 Validation: Packing Density Distributions

The packing density values of 11 shale materials derived from mineralogy and porosity measurements (i.e. Eq. (7.1)), provides a means of comparison with the packing densities we derive from a reverse analysis of the $(M, H)$ contact response of these materials. In fact, this comparison provides a formidable means to validate our approach. The validation is achieved in the following way:

1. For each tested sample, we determine the packing density distributions from the $(M, H)$ data set using the reverse algorithm presented in chapter 6. In this application, we consider the $(M, H)$ data sets of both orthogonal directions. The unknown solid properties are the solid’s strength properties ($c_s, \alpha_s$), which are assumed to be the same in orthogonal directions (isotropic strength behavior). In return, the asymptotic contact stiffness are different in orthogonal directions, and are fixed "close" to the values given by (6.4) and (6.5). Figure 7-2 shows a typical results of the $M_1(\eta), M_3(\eta)$ and $H(\eta)$ fit. The experimental points are randomly distributed on both sides of the model curves. More precisely, Figure 7-3 shows the distribution of the error between the experimental values and the fitted ones. As we can see, this distribution is close to a normal distribution, which a posteriori justifies the scaling model presented in chapter 6.

2. The packing density distribution we obtain for each sample span a large range of packing densities, underlining the highly heterogeneous nature of the porous clay phase in shales. In order to compare these packing density distribution with the single value packing density from mineralogy of each material, we determine the mean and the standard deviation of the packing density distribution vector $\text{Vect}_\eta = [\eta_1, ..., \eta_N]$. Results are reported in Figure 7-4 where the horizontal error bar, in each direction, represents one standard deviation.
Figure 7-2: Typical result of the indentation analysis program: $M_1(\eta), M_3(\eta)$ and $H(\eta)$ fit.
Figure 7-3: Result of the indentation analysis program: distribution of the error
Figure 7-4: Comparison between the packing density obtained from indentation analysis and from mineralogy of the distribution of packing density around the mean value.

The general trend in Figure 7-4 is an excellent agreement between the mean packing densities determined from two completely different means: mineralogy vs. contact response.

### 7.2 Level 0–Strength Properties

The second outcome of our analysis are the cohesion $c_s$ and the friction coefficient $\alpha_s$ of the elementary building block of shales; respectively the solid contact hardness (see Fig. 5-3 and Eq. (5.27)):

$$h_s = h_s (c_s, \alpha_s) \quad (7.2)$$
The validation of the packing density distributions seen before is a strong argument in favor of the relevance of these parameters to characterize the fundamental scale of shale's strength behavior. In this Section, we investigate, whether $c_s$, $\alpha_s$, and $h_s$ are truly intrinsic parameters, that is whether they are independent of the packing density.

### 7.2.1 Invariant Contact Hardness

We start with the contact hardness $h_s$. Figure 7-5 displays for the 11 shales the contact hardness versus their mean packing density. Two observations deserve particular attention:

- The contact hardness $h_s$ and the packing density are uncorrelated. In other words, $h_s$ is an intrinsic strength parameter that characterizes the strength behavior of the elementary building block of shales.

- Except for two values, all the samples have comparable values of $h_s$ comprised between 0.56 GPa and 0.80 GPa; despite their substantial difference in clay mineralogy:

$$ h_s = 0.69 \pm 0.09 \text{ GPa} \tag{7.3} $$

At first order, hardness $h_s$ of the solid phase appears as a material-invariant property.

### 7.2.2 Scaling of Friction with Packing Density

A further output of the algorithm, for each shale, is the solid friction coefficient $\alpha_s$ as a mean value of the combination of all best fits (Fig. 7-6). In contrast to the contact hardness $h_s$, however, the solid friction coefficient $\alpha_s$ varies strongly from shale to shale material from 0 to 0.41. Interestingly, by plotting the obtained values of the friction coefficient against the mean packing density of the sample, we observe a clear trend (Fig. 7-7): The friction, that is the pressure sensitivity of the elementary building block, decreases with the packing density increasing, approaching a zero-friction coefficient for the asymptotic solid state. In other words, the friction coefficient of shales is not a material invariant property, but depends on the (average) packing of the particles. Such a dependence advocates a geometrical origin of friction related
Figure 7-5: Distribution of the solid hardness, $h_s$, of all shales samples.
Figure 7-6: Histogram of the selected values of the solid friction coefficient, $\alpha_s$. [shale #4]

to asperities in the inter-particle space. Otherwise said, without voids there is no space for frictional effects to develop.

Hence, if the average packing of a specific shale is known, the friction coefficient can be determined. Considering a zero friction in an infinitely packed state ($\eta = 1$), and a certain saturation of the friction coefficient for low packing densities to its limit value (3.5), we propose the following relation:

$$\alpha_s = 1.2 \ (2 - 2\eta)^2 - 0.5 \ (2 - 2\eta)^5$$

(7.4)

(We also considered this relation in the hardness-packing density scaling, and checked whether this dependency would change the packing density distributions or the solid properties. We found that this effect was of second order).
Figure 7-7: Scaling of the solid friction, $\alpha_s$, with mean packing density.
7.2.3 Cohesion vs. Friction Relations

The last strength property we investigate is the solid cohesion \( c_s \). Since the contact hardness \( h_n \) is almost constant (see Fig. 7-5), it is readily recognized that the cohesion must increase with the mean packing density to counteract the decrease of the friction coefficient, \( \alpha_s = \alpha_s (\bar{\eta}) \). This is exactly what we find from the reverse analysis, as displayed in Figure 7-8 in form of a \( c_s - \alpha_s \) plot. One could argue that this increase of the cohesion with the mean packing density relates to the inter-particle space: as the system is looser packed the average distance between particles increases as well, which leads to a decrease of the interparticle bonds from which the cohesion originates. Figure 7-8 also displays the \( h_n = h_n (c_s, \alpha_s) \) relation (5.27) of the Drucker-Prager criterion for the mean contact hardness value (7.3); that is:

\[
c_s = \frac{h_n}{A} \times \frac{1}{\left(1 + B\alpha_s + (C\alpha_s)^3 + (D\alpha_s)^3\right)}
\]

with \( A = 4.76438, B = 2.5934, C = 2.1860, D = 1.6777 \). The asymptotic cohesion of the elementary building block of shale is obtained for \( \alpha_s \to 0 \), which corresponds to \( \bar{\eta} \to 1 \), that is:

\[
\lim_{\bar{\eta} \to 1} c_s = \frac{h_s}{A} = 0.14 \text{ GPa}
\]

7.2.4 Discussion

The results we obtain may be somewhat surprising: We first assumed, for each shale, the same solid strength properties, and find from a reverse analysis of 11 different shales of different mineralogy and porosity, that the friction coefficient and the solid cohesion depend on the mean packing density. To solve this puzzle, it is useful to remind ourselves of the micromechanical foundations of modeling the pressure sensitivity of a granular material with a bulk Drucker-Prager strength criterion. Indeed, as discussed in Section 3.2.2., a Drucker-Prager strength criterion represents at a smaller scale the strength behavior of a polycrystal with a Mohr-Coulomb interface strength criterion [41],[66]. The dependence of the Drucker-Prager friction coefficient on the mean packing density, therefore, hints towards the origin of the friction in this
Figure 7-8: Observed relation between the cohesion, $c_s$, and the solid friction coefficient of shales, $\alpha_s$. 

Experimental data for different shales

Adopted relation

Friction coefficient, $\alpha$

Solid cohesion, $c_s$ (normalized)
nanogranular material. It appears to originate from interfaces in the polycrystal structure of the clay minerals. Therefore, while $\alpha_s$ is not a material invariant property of clay particles and of their elementary frictional behavior, the scaling relation $\alpha_s$ vs $\eta$ appears to be an invariant characteristic of the porous polycrystal clay. Or otherwise said:

If we want to model a cohesive granular (polycrystal) material by a continuous cohesive-frictional model, we must adapt the friction coefficient of the solid phase to the packing density.

7.3 Towards Strength Prediction of Shale

The back-analysis of the solid-properties allows us to reduce the model parameters in a forward application to strength predictions of shales. Indeed, for a given clay packing density (determined from mineralogy, bulk density and/or porosity measurements), we can now determine—in a first approach—the solid friction coefficient from (7.4) and the solid cohesion from (7.5) and (7.6). This Section examines how those relations affect the overall strength domain at Level I and Level II of shales.

7.3.1 Level I—Predicted Strength Domain

Following the developments in Section 3.3, the strength domain of the porous clay phase can a priori be either elliptical or hyperbolic, depending on the value of the solid friction coefficient (Eq. (3.52)). On the other hand, if we use, for the polycrystal morphology, the $\alpha_s - \eta$ relation (7.4) in (3.62), we readily find that the strength domain of the porous clay phase is always elliptical. This is illustrated in Figure 7-9 which shows, for the clay cohesion (7.6), the evolution of the strength domain with the packing density. As the indentation technique probes the strength properties of materials in compression, we only report strength domains in the region where $\Sigma_m < 0$: In the asymptotically packed state ($\eta = 1$), where the friction is zero, the strength behavior takes a purely cohesive form described by a Von-Mises model. In return, an increase in the voids has three effects: (i) the Von-Mises strength criterion becomes an ellipse (centered around the origin), (ii) the decrease in cohesion leads to an overall shrinkage of the ellipse, lowering in particular the overall maximum shear (ellipse summit); and (iii) the increase
in friction leads to a shift of the center of the ellipse along the negative hydrostatic axis, which is partly compensated by the decrease in cohesion for low packing densities.

### 7.3.2 Level II—Predicted Strength Domain

This section examines the effect of the addition of rigid inclusions on the macroscopic strength domain. Given the elliptical shape of the strength domain at Level I, the strength domain at Level II is also elliptical. We derived this relation in Section 3.4. Furthermore, the Level I polycrystal morphology for shales reduces possible permutations to four that relate to the Level II morphology (Self-Consistent vs. Mori-Tanaka) and interface conditions (adherence vs. slippery):

<table>
<thead>
<tr>
<th>Level II Interface Condition</th>
<th>Level II Morphology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adherence (IA)</td>
<td>PA - SC  PA - MT</td>
</tr>
<tr>
<td>Slippery (IS)</td>
<td>IS - SC  IS - MT</td>
</tr>
</tbody>
</table>
Effect of the Level II–Homogenization Scheme

Figure 7-10 displays the enlargement of the elliptical strength domain of a porous clay phase of packing density $\eta = 0.7$ by the addition of perfectly adherent rigid inclusions of volume fraction $f_{inc} = \{0.2, 0.4\}$, predicted respectively by the Mori-Tanaka scheme (Fig. 7-10(a)) and the self-consistent scheme (Fig. 7-10(b)). As already observed in Section 5.3.2 for the hardness-to-cohesion ratio, the self-consistent scheme compared to the Mori-Tanaka scheme amplifies the effects of inclusions on the strength domain, particularly for inclusion volume fractions close to 0.5 (for which the strength domain would be infinite). Hence, the higher the disorder in the material system at Level II, the more pronounced the reinforcing effects of rigid inclusions.

Effect of the Interface Condition

Figure 7-11 display the change of the elliptical strength domain of the porous clay phase due to the addition of rigid inclusions with slippery interfaces, for both the Mori-Tanaka scheme (Fig. 7-11(a)) and the Self-Consistent scheme (Fig. 7-11(b)). For this interface condition, we confirm that a disordered morphology (represented by the self-consistent scheme) amplifies the effects of rigid inclusions compared to a clear matrix-inclusion morphology (represented by the Mori-Tanaka scheme). Furthermore, as one expects from a slippery interface condition, the strength enhancement is much smaller than if one had a perfect adherent interface. An interesting observation is that the self-consistent scheme predicts an overall increase of the size of the ellipse due to the addition of inclusions (Fig. 7-11(b)), while the addition of slippery inclusions in the Mori-Tanaka case actually entails an increase along the hydrostatic axis and a decrease along the deviatoric axis.

This effect is shown in Figure 7-12 which plots the uniaxial compressive strength $\left(\Sigma_m = \frac{1}{3} \Sigma; \Sigma_d = \sqrt{2J_2} = \sqrt{\frac{2}{3} |\Sigma|}\right)$ for the four possible configurations as a function of the inclusion volume fraction. It turns out that the Mori-Tanaka scheme predicts indeed a weakening of the uniaxial strength with increasing slippery rigid inclusions.
Figure 7-10: Influence of the perfectly adherent rigid inclusions at Level II. Figures generated starting from a porous clay phase with \( \eta = 0.7 \). (a) using a Mori-Tanaka scheme. (b) using a Self-Consistent scheme.
Figure 7-11: Influence of the rigid inclusions with slippery interfaces at Level II. Figures generated starting from a porous clay phase with $\eta = 0.7$. (a) using a Mori-Tanaka scheme. (b) using a Self-Consistent scheme.
Figure 7-12: Evolution of the compressive strength with the volume fraction of rigid inclusions.
7.4 Chapter Summary

In this chapter, we applied the novel tools of indentation analysis based on multiscale strength homogenization to data sets coming from experiments on eleven shale materials. The reverse algorithm was found to give accurate values of the packing density distribution as it matches the estimation obtained from other experimental techniques. We identified a strength invariant, the contact hardness $h_s$, and an intrinsic scaling of the friction coefficient and the cohesion with the mean packing density. On this basis, it is possible to predict the strength domain of shales based on only two parameters: the clay packing density and the inclusion volume fraction. A first application to the Level II strength domain shows the potential of this approach, which—once fully validated—could become an engineering tool for strength prediction of shales based on a minimum numbers of material parameters of clear chemo-physical origin.
Part V

Conclusion and Perspectives
Chapter 8

Summary of Results and Future Perspectives

Despite their ubiquitous presence as sealing formations in hydrocarbon bearing reservoirs affecting many fields of exploitation, the link between mineralogy composition, microstructure, and mechanical strength properties of shale has long time been an enigma that has deceived many decoding attempts from experimental and theoretical sides. Based on a highly reductionist multiscale homogenization approach of the strength properties of shale, which condenses mineralogy, bulk density and porosity into two quantities, namely clay packing density and inclusion volume fraction, we find that it is possible to reduce the complexity of shale materials to a scale where the strength behavior is governed by shale invariant strength properties, and to upscale this behavior from the nanoscale to the macroscale of engineering strength prediction.

8.1 Summary of Main Findings

With the multi-scale model of shale in mind (Fig. 3-1), this investigation provides strong evidence for the following conclusions:

1. Level ‘0’: The fundamental building block of shale strength behavior is a polycrystal cohesive-frictional material. We come to this conclusion from the backanalysis of nanoin- dentation results of 11 different shale materials, which show that the particle-to-particle
contact hardness $h_s$ is in first order constant for all shale materials, i.e. independent of mineralogy and porosity; while the Drucker-Prager cohesion $c_s$ and the friction coefficient $\alpha_s$ depend on the mean packing density $\bar{\eta}$ and are therefore shale dependent. We summarize these findings in the following intrinsic relations:

$$h_s = 0.69 \pm 0.09 \text{ GPa} \quad (8.1)$$
$$\alpha_s = 1.2 \, \left(2 - 2\bar{\eta}\right)^2 - 0.5 \, \left(2 - 2\bar{\eta}\right)^5 \quad (8.2)$$
$$c_s = \frac{h_s}{A} \times \frac{1}{\left(1 + B\alpha_s + (C\alpha_s)^3 + (D\alpha_s)^{10}\right)} \quad (8.3)$$

with $A = 4.76438$, $B = 2.5934$, $C = 2.1860$, $D = 1.6777$. For the theoretical solid state, $\bar{\eta} \to 1$, the elementary building block is purely cohesive (i.e. frictionless), having a Drucker-Prager cohesion $\lim c_s = 0.14 \pm 0.02 \text{ GPa}$, which translates into a uniaxial strength of $Y = 0.25 \text{ GPa}$.

2. Level 'I': The porous clay phase is a nanogranular material. Due to the intrinsic relations (8.1)-(8.3), we find that the Level I strength domain is described by an elliptical strength criterion, which is a sole function of the clay packing density $\eta$. We come to this conclusion by the application of an original strength homogenization model that covers both the elliptical and hyperbolic case, to shale nanoindentation analysis.

3. Level 'II': The effect of rigid inclusions to the porous clay phase depends critically on the Level II morphology and the interface condition between inclusions and matrix, a dependency that supports the simple idea that the overall strength properties of a material are controlled by the weakest constituent: The general trend is that a disordered morphology and perfect adherence between inclusion and matrix, entail a more substantial increase of the strength domain than an ordered matrix-inclusion morphology and imperfect slippery interface conditions. A combination of a matrix-inclusion morphology with slippery interface conditions can even lead to a shear strength loss compared to the level I properties.

While the Level 'I' and Level 'II' results are supported by a comprehensive nanoindentation analysis of different shale materials, the Level 'II' results are at this stage preliminary in the
sense that they require future validation.

8.2 Research Contributions

The multiscale strength homogenization approach we here propose for shales removes limitations of previous approaches. On the way, the following contributions were made:

1. To the field of strength homogenization of porous materials, an original step-to-step non-linear yield design homogenization procedure was proposed, that translates the Linear Comparison Composite Theory (Chapter 2) into a workable model for shale multiscale strength homogenization. This allowed us to derive the expression of the strength criterion of a porous composite material made of a Drucker-Prager solid phase, voids and inclusion for any solid packing density (Chapter 3). Compared to previous contributions based on the effective strain rate approach [5],[3],[38], the model we propose covers both the elliptical and the hyperbolic case, and removes the restriction to small friction coefficients and associated packing densities below the critical threshold that separates the elliptical from the hyperbolic case. The procedure here proposed is sufficiently flexible that it can be employed to many other situations; for instance to the strength homogenization of an N-phase composite with finite strength (Appendix 4).

2. To the field of nanoindentation analysis of heterogeneous materials, the novel hardness-to-packing density scaling relations extend previous work [19],[20] to a larger range of possible packing densities, that covers in a continuous fashion the elliptical and the hyperbolic case (Chapter 5). Furthermore, scaling relation were also obtained for Level II, incorporating the influence of rigid inclusions (Chapter 5). Implementation of these relations in a reverse analysis algorithm (Chapter 6) provides a versatile means to probe the microstructure of any cohesive-frictional porous material, and to separate constituent strength properties \((c_s,\alpha_s)\) from microstructure \((\eta,\eta_0)\) in indentation analysis of porous materials. Given the difficulty of estimating the porosity of porous materials with classical methods, the reverse algorithm provides a new non-intrusive way to determine the porosity of nanogranular materials from their nanomechanical contact response.
3. To the field of geomechanics in general and the GeoGenome project in particular, the identification of the intrinsic relations (8.1)-(8.3) for shales is of critical importance. On the one side, our contribution confirms that shales are nanogranular materials, and suggests that its elementary clay building block is a cohesive-frictional polycrystal. On the other hand, with a view on strength prediction for shale, relations (8.1)-(8.3) reduces the number of input parameters for strength prediction to two: clay packing density $\eta$ and inclusion volume fraction $f_{inc}$. This opens new perspectives for strength prediction of shale based on only mineralogy and porosity information.

8.3 Current Limitations and Future Perspectives

There are some inherent limitations of our approach which relate to the application of yield design for indentation analysis: One restriction of our approach relates to the assumption of the normality rule, applied for both strength homogenization and hardness simulations. This principle of maximum plastic work is at the very basis of the yield design formulation and cannot capture a possible non-associated flow behavior. In such cases, advanced finite element simulations are required. A similar remark can be made for contact friction and strain hardening effects, which we ignore in our yield design solutions.

It could also be argued that the finite element simulations developed in this thesis do not capture piling-up or sinking-in phenomena, as our yield design formulation evaluates the dissipation capacity of a material system for a fixed geometry. Indeed, in the simulations we assume the surface of the indenter to be flat, which is far from what is observed in indentation tests of shales (see, for instance, Fig. 7-1). However, compared to the material bulk volume that contributes to the overall dissipation capacity, the additional contribution of the pile-up volume is expected to be of second order [20]. Of course, the piling-up or sinking-in phenomena cannot be neglected in the evaluation of the hardness value from its definition (4.2), which is the input to the reverse analysis using the proposed hardness-scaling relations. Otherwise said, like all indentation procedures, the successful determination of the strength properties from indentation tests relies on the determination of the correct projected contact area.

Finally, our contribution is a modest yet important step forward towards a comprehen-
sive multiscale approach to the complexity of shale's strength behavior, which still need to be achieved. In order to close the loop between the nanomechanical behavior and the macroscopic strength behavior, future research may provide answers to the following questions:

1. At level ‘0’ – What is the origin of clay cohesion, and how does it relate to mineral properties? While our approach hints towards a polycrystal structure of the elementary clay building block, the link between the clay packing, pore size and mineralogy needs still to be established. Since nanoindentation on shale cannot access the individual clay mineral properties and interface properties, it is expected that advanced atomistic simulations may be able to shed light on this link, and to identify the origin of the clay cohesion. A similar remark applies to the found dependence (8.2) of the friction angle on the packing density, which needs to be confirmed for other materials that span a large range of packing densities.

2. At Level I – Does particle shape matter? In our approach we assumed a percolation threshold of $\eta_0 = 0.5$, which appears to be a good match for high clay packing densities. On the other hand, as it is well known, clay particles are not spherical but oblate ellipsoids. While this particle shape no-doubt plays a second order role for high packing densities, it may however, affect the strength response at packing densities around and below $\eta < 0.5$. Indeed, recent results in linear micromechanics showed that the self-consistent percolation threshold decreases when the aspect ratio deviates from the spherical case [89], and a similar result is expected for the strength case. Future work, therefore, may want to consider a clay aspect ratio in the Level I strength homogenization procedure. It is expected that the proposed homogenization procedure based on the Linear Comparison Composite could be adapted to accomodate the particle shape.

3. At Level II – What are the true interface conditions of the silt inclusions in shale? Answering this question will require a comprehensive comparison of the predicted strength domain with triaxial strength test results on a large variety of shale materials. Such an in-depth study is necessary in order to refine and validate our strength prediction model.

Once these questions will be solved, there is no doubt that progress in nanoscience and nanoengineering of shale will translate into day-to-day engineering applications.
Part VI

Appendices
Appendix A

Linear homogenization theory

This appendix introduces the main ideas of homogenization in the linear case. The notion of homogeneous stiffness tensor is exposed as well as the main tools for its estimation. As it plays a key role in Chapters 2 and 3, the variational formulation of the problem is established and we show how it can be used to derive bounds for the homogeneous stiffness. It is inspired from [5], [84].

A.1 Introduction

Generally speaking, a classical problem of Continuum Mechanics would consider a homogeneous material with a given shape and subjected to a given loading and boundary conditions. It would look, in particular, for the displacement and stress fields and would require the prior knowledge of the behavior of the solid, which is characterized by some stiffness and strength properties. However, if we have a closer look at the material and observe it at the microscopic scale, very often we observe that the material is not rigorously homogeneous and is in fact composed of different phases with distinct properties. This is the case, for instance, of most metals who at the scale of a few microns exhibit a polycrystalline structure.

The stiffness and strength properties used in the homogeneous continuum mechanics problem are in fact "averages" of the different phases present at the microscale and depend, in particular, on their mechanical properties and spacial arrangement. The observation that the material is heterogeneous at the microscale but homogeneous at the macroscale suggests that an
"averaging" process occurs during the transition between these two scales of observation. The study of this phenomenon is the focus of the theory called Homogenization. It takes as input some morphological and mechanical information on an heterogeneous material and computes the resulting effective properties observed at a larger scale. It forms the basis for the development of new composite materials such as fiber reinforced polymers, plastic-impregnated textiles or metal matrix composites. However, this theory also applies to the study of any heterogeneous material and in particular geomaterials.

It is important to note that this homogenization phenomenon can be observed only when the typical dimension of heterogeneities is much smaller than the scale of study. Indeed, we must be able to define a Representative Volume Element (RVE, typical dimension $\mathcal{L}$) who captures the average behavior of all the heterogeneities (typical dimension $d$) and this RVE also has to be much smaller than the size of the solid studied in the framework of Continuum Mechanics (typically $h$).

$$d \ll \mathcal{L} \ll h$$  \hspace{1cm} (A.1)

If we account for at least one order of magnitude for each of these relation we obtain that the heterogeneities have to be at least 100 times smaller than the size of the system studied. As we mentioned earlier, the materials considered in this thesis are heterogeneous but we can assume that the scale separability condition holds during an indentation experiment. Indeed, the size of voids is typically of the order of $20$ to $100 \mu m$ and the size of the region activated during a typical indentation is $10 \mu m$.

A.2 Change of scales

A.2.1 Modelling

General case

We consider a heterogeneous material made of $N$ phases \{i = 1..N\} having a linear elastic behavior characterized by their stiffness tensor $C_i$. Each phase is considered as homogeneous and may be anisotropic. We don't assume any property on the spacial distribution of these phases. We allow for discontinuities in the displacement at the interfaces, however, these discontinuities
Figure A-1: A typical heterogeneous material. The choice of two different regions of the material leads to two mechanically equivalent RVEs.

cannot be normal to the surface.

We assume that the different phases have a characteristic size and that, by considering a much larger volume, it is possible to obtain a representative view of the material. Then we can define a Representative Volume Element (RVE) that has to meet two requirements:

- It must be mechanically equivalent whether we consider it around two different points in the material.
- Its dimensions must be much larger than the characteristic size of the heterogeneities.

Figure A-1 sketches a typical 2 phases composite material respecting this condition. A material with periodic microstructure is also a good example of material subject to our study (the RVE will be taken with dimensions much larger than the unit cell). A material with random microstructure and with a clearly defined maximal dimension for the heterogeneities is also subject of our study. We will consider in this case a much larger volume than this maximal dimension. However, a material in which there is no clear limitation on the size of the heterogeneities cannot exhibit a homogeneous behavior at the macroscale. That emphasizes the importance of the definition of a typical dimension of the heterogeneities $d$.

The dimension of the RVE, $\mathcal{L}$, has to be much larger than the one of heterogeneities:

$$d \ll \mathcal{L}$$  \hspace{1cm} (A.2)
The "averaging phenomenon" of homogenization occurs between these two length scales $d$ and $\mathcal{L}$. The RVE represents the homogenized material and its associated mechanical properties are the effective ones of the composite material. This allows for a subsequent analysis based on continuum mechanics and considering a homogeneous material. In this study at the macroscale, the size of the RVE must be much smaller than the one of the system, say $h$, since a RVE is supposed to represent a point. That leads to a second condition:

$$\mathcal{L} \ll h$$  \hfill (A.3)

Finally, we must impose a condition on the loading, namely a characteristic length of its fluctuation. Indeed, the notion of RVE would lose its whole effectiveness if we were to study a problem where a structure is subjected to a loading with important fluctuations below the scale of the RVE. If $\sigma$ is the stress and $f$ the externally applied load density, this regularity condition also implies that:

$$\sigma \propto h f$$  \hfill (A.4a)

$$\sigma \gg \mathcal{L} f$$  \hfill (A.4b)

### A.2.2 Fields statistics

Based on the previous assumption of scale separability, we consider two continuum mechanics problems relative to the two scales of our problem. In the first one, the overall dimensions of our system are the ones of the RVE, $\mathcal{L}$, and the dimensions of a point are much smaller than $d$, such that we can consider the heterogeneities as continuous solids. In the second problem, the overall dimensions of our system are the ones of the macroscopic system, $h$, and each RVE is assimilated to a point.

The quantities of the microscopic problem will be noted with lower-case and the one of the macroscopic problem with upper-case:
The macroscopic quantities are defined as the local average of the microscopic ones. If $\Omega(X)$ is the RVE centered at point $X$, then for any quantities $A(X)$ and $a(\mathbf{x})$, we have:

$$A(X) = \langle a(\mathbf{x}) \rangle_{\Omega(X)} = \frac{1}{|\Omega|} \int_{\Omega(X)} a(\mathbf{x}) \, d\mathbf{x}$$  \hspace{1cm} (A.5)

If we take the derivative of relation (A.5), we obtain:

$$\frac{\partial A(X)}{\partial X_i} = \frac{1}{|\Omega|} \int_{\partial \Omega(X)} a(\mathbf{x}) \Gamma_i \, dS = \frac{1}{|\Omega|} \int_{\Omega(X)} \frac{\partial a}{\partial x_i} \, d\mathbf{x}$$  \hspace{1cm} (A.6)

This can be extended in the presence of discontinuity in the field $a(\mathbf{x})$:

$$\frac{\partial A(X)}{\partial X_i} = \frac{1}{|\Omega|} \int \left\{ \frac{\partial a}{\partial x_i} \right\} d\mathbf{x} + \frac{1}{|\Omega|} \int_{\Pi \cap \Omega(X)} \left[ \frac{\partial a}{\partial x_i} \right] n_i \, d\mathbf{n}$$  \hspace{1cm} (A.7)

where $\Pi$ is the surface of discontinuity and $\left\{ \frac{\partial a}{\partial x_i} \right\}$ is the distribution defined outside of the discontinuities by the integrable function $\frac{\partial a}{\partial x_i}$.

**Homogenization of the strain**

As suggested by formula (A.5), the macroscopic strain is expressed by:

$$\mathbf{E}(X) = \langle \varepsilon(\mathbf{x}) \rangle_{\Omega(X)} = \frac{1}{|\Omega|} \int_{\Omega(X)} \varepsilon(\mathbf{x}) \, d\mathbf{x}$$  \hspace{1cm} (A.8)

In the presence of discontinuities, it reads:

$$\mathbf{E}(X) = \frac{1}{|\Omega|} \int_{\Omega(X)} \{ \varepsilon \}(\mathbf{x}) \, d\mathbf{x} + \frac{1}{|\Omega|} \int_{\Pi \cap \Omega(X)} \frac{1}{2} \left( \left[ \frac{\partial \varepsilon}{\partial x_i} \right] \otimes n + n \otimes \left[ \varepsilon \right] \right) \, d\mathbf{n}$$  \hspace{1cm} (A.9)

\(^1\langle \mathbf{x} \rangle = \bar{\mathbf{x}}\)
A very interesting property of the macroscopic strain is that it only depends on what happens on the boundary of the RVE. Indeed, the use of the divergence theorem in the previous relation yields:

$$\mathbf{E}(x) = \frac{1}{|\Omega|} \int_{\partial \Omega(x)} \frac{1}{2} \left( \xi(x) \otimes \mathbf{n} + \mathbf{n} \otimes \xi(x) \right) \, dS$$  \hspace{1cm} (A.10)

The macroscopic strain depends only on the displacement on the boundary of the RVE.

**Homogenization of the stress**

The macroscopic stress is given by:

$$\Sigma(x) = \langle \sigma(\mathbf{x}) \rangle_{\Omega(x)} = \frac{1}{|\Omega|} \int_{\Omega(x)} \sigma(\mathbf{x}) \, d\mathbf{x}$$  \hspace{1cm} (A.11)

Similarly to the macroscopic strain $\mathbf{E}$, we can show that $\Sigma$ only depends on what happens on the boundary of the RVE. Indeed, if $\mathbf{f}$ is the externally applied load density:

$$\text{div}(\mathbf{x} \otimes \sigma(\mathbf{x}))_{ij} = \frac{\partial (x_i \sigma_{jk})}{\partial x_k} = \frac{\partial x_i}{\partial x_k} \sigma_{jk} + \frac{\partial \sigma_{jk}}{\partial x_k} x_i = \sigma_{ji} + f_j x_i$$  \hspace{1cm} (A.12)

but since $x_i$ is of the order of $\mathcal{L}$ and recalling condition (A.4b), the second term in the previous equation is negligible such that:

$$\text{div}(\mathbf{x} \otimes \sigma(\mathbf{x})) = \sigma(\mathbf{x})$$  \hspace{1cm} (A.13)

Then, making use of the divergence theorem,

$$\Sigma(x) = \frac{1}{|\Omega|} \int_{\Omega(x)} \sigma(\mathbf{x}) \, d\mathbf{x} = \frac{1}{|\Omega|} \int_{\partial \Omega(x)} \mathbf{x} \otimes \sigma(\mathbf{x}) \cdot \mathbf{n} \, dS$$  \hspace{1cm} (A.14)

which can be extended to the case with discontinuities because of the classical jump condition over the stress field:

$$[[\sigma]] \cdot \mathbf{n} = 0 \quad \text{on } \Pi$$  \hspace{1cm} (A.15)
A.2.3 Homogeneous stiffness tensor

Problem with homogeneous boundary conditions

As mentioned in the introduction, the goal of linear homogenization is to find the homogeneous stiffness tensor of a given composite. That means that we want to find the relation between the macroscopic strain $\mathbf{E}$ and the macroscopic stress $\mathbf{\Sigma}$. To achieve that, we are going to study two model problems of the RVE. In the first problem, displacement at the boundary will be prescribed whereas in the second one, stresses will be prescribed.

We consider that these boundary conditions are homogeneous. For fixed $\mathbf{E}$ and $\mathbf{\Sigma}$, it means that:

- If displacement is prescribed,
  $$\xi = \mathbf{E} \cdot \mathbf{x} \quad \text{on } \partial \Omega \quad (A.16)$$

- If stresses are prescribed,
  $$\mathbf{\sigma} \cdot \mathbf{n} = \mathbf{\Sigma} \cdot \mathbf{n} \quad \text{on } \partial \Omega \quad (A.17)$$

These boundary conditions translate the idea that the macroscopic state of stress does not vary much over a RVE. In addition, based on relations (A.10) and (A.14), they ensure that the average of the strain and of the stress are indeed $\mathbf{E}$ and $\mathbf{\Sigma}$.

We can also neglect the influence of the externally applied load density. The change in stress it would induce is of the order of $\mathcal{L} f$ which is negligible compared to $\mathbf{\Sigma}$ (relation A.4b). That leads to replacing the classical equation

$$\text{div} (\mathbf{\sigma}) + f = 0 \quad (A.18)$$

by the easier one:

$$\text{div} (\mathbf{\sigma}) = 0 \quad (A.19)$$
This property will allow us to utilize Hill’s lemma:

\[
\begin{align*}
\text{div} (\sigma) &= 0 \\
\xi &= \mathbf{E} \cdot \mathbf{x} \quad \text{on} \ \partial \Omega \\
\text{or} \quad \sigma \cdot \mathbf{n} &= \Sigma \cdot \mathbf{n} \quad \text{on} \ \partial \Omega
\end{align*}
\]

\[\implies \langle \sigma : \varepsilon \rangle = \langle \sigma \rangle : \langle \varepsilon \rangle \quad \text{(A.20)}\]

Finally, we can summarize the equations of the problem:

\[
\begin{align*}
\text{div} (\sigma) &= 0 \quad \text{in} \ \Omega \\
\sigma &= \mathbf{C}_1 : \varepsilon \quad \text{in} \ \Omega_i \\
\varepsilon &= \frac{1}{2} (\text{grad} \xi + '\text{grad} \xi) \quad \text{in} \ \Omega \\
\xi &= \mathbf{E} \cdot \mathbf{x} \quad \text{on} \ \partial \Omega \\
\text{or} \quad \sigma \cdot \mathbf{n} &= \Sigma \cdot \mathbf{n}
\end{align*}
\]

\[\text{(A.21a)} \quad \text{(A.21b)} \quad \text{(A.21c)} \quad \text{(A.21d)}\]

**Localization tensors and homogeneous stiffness tensor**

Because of the linearity of the problem, there is a linear relation between the fields \(\varepsilon (\mathbf{x})\) and \(\sigma (\mathbf{x})\) solution to the equations of the problem and the boundary conditions \(\mathbf{E}\) and \(\Sigma\).

If displacement are prescribed, we can write:

\[
\varepsilon (\mathbf{x}) = \mathbf{A} (\mathbf{x}) : \mathbf{E} \quad \text{(A.22)}
\]

where \(\mathbf{A} (\mathbf{x})\) is called strain concentration tensor. Then the stress field reads:

\[
\sigma (\mathbf{x}) = \mathbf{C} (\mathbf{x}) : \mathbf{A} (\mathbf{x}) : \mathbf{E} \quad \text{(A.23)}
\]

So

\[
\Sigma = \langle \sigma (\mathbf{x}) \rangle_\Omega = \langle \mathbf{C} (\mathbf{x}) : \mathbf{A} (\mathbf{x}) \rangle_\Omega \cdot \mathbf{E} \quad \text{(A.24)}
\]

and we can define the homogeneous stiffness tensor by:

\[
\mathbf{C}^{\text{hom}} = \langle \mathbf{C} (\mathbf{x}) : \mathbf{A} (\mathbf{x}) \rangle_\Omega \quad \text{(A.25)}
\]
In the case of discontinuities in displacement, we write \( \{ A(x) \} \) the localization tensor distribution defined outside of the discontinuities and \( a(x) \) the surface localization tensor distribution on the surface of discontinuities:

\[
\frac{1}{2} \left( \left[ [e] \right](x) \otimes n + n \otimes \left[ [e] \right](x) \right) = a(x) : E \tag{A.26}
\]

Then, similarly to (A.7), the localization tensor has two terms:

\[
A(x) = \{ A(x) \} + a(x) \tag{A.27}
\]

However, the macroscopic stress tensor is not affected by the discontinuity and reads:

\[
\Sigma = \langle \sigma(x) \rangle_\Omega = \langle C(x) : \{ A(x) \} \rangle_\Omega : E \tag{A.28}
\]

so the homogeneous stiffness tensor is defined in this case by:

\[
C^{\text{hom}} = \langle C(x) : \{ A(x) \} \rangle_\Omega \tag{A.29}
\]

Remark 1  The concentration tensor \( A \) does not necessarily possess major symmetry: in general \( A_{ijkl} \neq A_{klij} \). However, since it acts on symmetric second order tensors, it has the minor symmetry: \( A_{ijkl} = A_{jikl} \) and \( A_{ijkl} = A_{ijk} \).

Remark 2  Because of its definition (A.22), the mean of the concentration tensor \( A \) is equal to the fourth order identity tensor:

\[
\langle A(x) \rangle_\Omega = I \tag{A.30}
\]

Remark 3  Since the value of \( C(x) \) is known from the modeling of the material, \( C(x) \) is a piecewise constant function: \( C(x) = C_i \) in \( \Omega_i \), the critical part in the estimation of the homogeneous stiffness tensor will be the determination of the strain concentration tensor \( A(x) \), which incorporates all the information on the properties of the system and its morphology.

Remark 4  Since \( C(x) \) is constant in each phase, we can take it out from the mean operator.
and we get:

\[ C^{\text{hom}} = \sum_i \phi_i C_i : \langle A'(\mathbf{x}) \rangle_{\Omega_i} \]  

(A.31)

where \( \phi_i \) is the volume fraction of phase \( i \). That suggests that we don't need to know the value of \( A'(\mathbf{x}) \) in each point of the system. We just need to know its mean in each phase.

Similarly, if the loading is prescribed, we can write:

\[ \sigma(\mathbf{x}) = B(\mathbf{x}) : \Sigma \]  

(A.32)

where \( B(\mathbf{x}) \) is the stress concentration tensor. We can define the homogeneous compliance tensor by:

\[ S^{\text{hom}} = \langle S(\mathbf{x}) : B(\mathbf{x}) \rangle_{\Omega} \]  

(A.33)

It is important to note that the homogeneous boundary conditions that we have imposed are not the fruit of a reasoning on the change of scale and are probably not encountered in reality. However, they allow us to formulate properly the mechanical study of the RVE and are compatible with the mean quantities. We may also add that there is no reason for the solutions to two problems to be the same. However, homogenization would have no meaning if the homogeneous stiffness tensors was strongly dependant on the actual conditions at the boundary of the RVE. In fact, these two problems lead to very close estimations of the macroscopic stiffness. In 1967, R. Hill [56] showed that provided that the scale separability conditions are enforced, the inverse of the homogeneous compliance tensor (A.33) tends to the homogeneous stiffness tensor (A.25). He also quantified the error as a function of the ratio \( \frac{d}{L} \):

\[ S^{\text{hom}} : C^{\text{hom}} = I + \mathcal{O} \left( \left( \frac{d}{L} \right)^3 \right) \]  

(A.34)

That forms a good argument proving that the homogeneous stiffness found by this procedure is an accurate representation of the behavior of the material at the macroscopic scale.

**Remark 5** We could also have opted for a definition of the homogeneous stiffness based on energy considerations. In the case of displacement boundary conditions, the equivalence between
the microscopic and the macroscopic energy would read:

$$\langle \varepsilon : C : \varepsilon \rangle_\Omega = \langle E : tA : C : A : E \rangle_\Omega \overset{def}{=} E : C^{\text{hom}} : E$$  \hspace{1cm} (A.35)

$$\implies C^{\text{hom}} = \langle tA : C : A \rangle_\Omega$$  \hspace{1cm} (A.36)

which at first sight does not seem equivalent to definition (A.25). However, for fixed \( \{i, j, p, q\} \) the component \( C_{ijpq}^{\text{hom}} \) reads:

$$C_{ijpq}^{\text{hom}} = \left\langle \left( tA \right)_{ijkl} C_{ikmn} A_{npq} \right\rangle_\Omega = \left\langle k_{ij} C_{ikmn} A_{npq} \right\rangle_\Omega$$  \hspace{1cm} (A.37)

which can be interpreted as the product:

$$C_{ijpq}^{\text{hom}} = \langle \varepsilon_2 : C : \varepsilon_1 \rangle_\Omega$$  \hspace{1cm} (A.38)

with \( \varepsilon_1 \) defined by \( \varepsilon_1(\varepsilon) = A(\varepsilon) : \tilde{E}_1 \) where \( \tilde{E}_1 = \frac{1}{2} \delta_p \delta_q (e_p \otimes e_q + e_q \otimes e_p) \) and \( \varepsilon_2 \) defined by \( \varepsilon_2(\varepsilon) = A(\varepsilon) : \tilde{E}_2 \) where \( \tilde{E}_2 = \frac{1}{2} \delta_i \delta_j (e_i \otimes e_j + e_j \otimes e_i) \). In that case, \( \sigma_1(\varepsilon) = C : \varepsilon_1(\varepsilon) \) is the stress field solution to the problem with displacement boundary conditions defined by \( \tilde{E}_1 \). Therefore, it is divergence free. \( \varepsilon_2 \) is the strain field solution to the problem with displacement boundary conditions defined by \( \tilde{E}_2 \). Consequently, the application of Hill’s lemma yields:

$$C_{ijpq}^{\text{hom}} = \left\langle \tilde{E}_2 : tA(\varepsilon) \right\rangle_\Omega : \left\langle C : A(\varepsilon) : \tilde{E}_1 \right\rangle_\Omega \hspace{1cm} (A.39)$$

$$= \tilde{E}_2 : \left( C : A(\varepsilon) \right)_\Omega : \tilde{E}_1$$

$$= \left( \langle C : A(\varepsilon) \rangle_\Omega \right)_{ijpq}$$

where use has been made of the property: \( \langle A(\varepsilon) \rangle_\Omega = I \).

A similar reasoning leads to the same result in the case of prescribed loading at the boundary.

**Remark 6** This equivalence shows that the homogeneous stiffness tensor has both the minor and major symmetry classically required by the theory of continuum mechanics (Eq. (A.37))
A.3 Eshelby inclusion problem and associated estimates

As we mentioned, the determination of the homogeneous stiffness of a given linear composite is achieved through the determination of the strain or stress concentration tensor. In this section, we show how the study of a single inclusion by Eshelby can be used to elaborate estimates for the strain concentration tensor.

A.3.1 Eshelby's isolated inclusion problem

General case

In 1957, J. D. Eshelby [40] considered the case of an isolated ellipsoidal inclusion (I) with constant elasticity tensor $C_1$ embedded in an infinite medium with a different elasticity tensor $C_0$ and subjected to a uniform strain $E^\infty$ at infinity (Fig A-2).

The domain occupied by the inclusion is defined by:

$$I = \{ \xi \in \mathbb{R}^3 | \xi \left( A A \right)^{-1} \xi \leq 1 \}$$  \hspace{1cm} (A.40)

where $A$ is a second order tensor. If $\xi_1, \xi_2, \xi_3$ are the directions of the main axis and $a_1, a_2, a_3$
are the half lengths of the axis, then:

\[ \mathbf{A} = a_1 \mathbf{e}_1 \otimes \mathbf{e}_1 + a_2 \mathbf{e}_2 \otimes \mathbf{e}_2 + a_3 \mathbf{e}_3 \otimes \mathbf{e}_3 \]  \hspace{1cm} (A.41)

and the equation of the ellipsoid is:

\[ \left( \frac{x_1}{a_1} \right)^2 + \left( \frac{x_2}{a_2} \right)^2 + \left( \frac{x_3}{a_3} \right)^2 \leq 1 \]  \hspace{1cm} (A.42)

The derivation of the solution uses polarization fields. We will introduce them in the section on the variational formulation; but here is a summary of the main results:

- The strain field inside the inclusion is constant.

- The value of the strain inside the inclusion is:

\[ \forall \mathbf{y} \in \mathcal{I}, \quad \mathbf{\varepsilon} (\mathbf{y}) = (\mathbf{I} + \mathbb{P}_0 : (\mathbf{C}_1 - \mathbf{C}_0))^{-1} : \mathbf{E}^\infty \]  \hspace{1cm} (A.43)

where:

\[ \mathbb{P}_0 = \frac{\det \mathbf{A}}{4\pi} \int_{|\mathbf{y}|=1} \frac{\mathbf{y} \otimes (\mathcal{L} \mathbf{C}_0 \mathbf{y})^{-1} \otimes \mathbf{y}}{3} dS \]  \hspace{1cm} (A.44)

**Case of a spherical inclusion**

If the reference medium is isotropic,

\[ \mathbf{C}_0 = 3\kappa_0 \mathbb{J} + 2\mu_0 \mathbb{K} \]  \hspace{1cm} (A.45)

and the inclusion is a sphere (i.e. \( \mathbf{A} = \mathbb{1} \)), then

\[ \mathbb{P}_0 = \frac{1}{3\kappa_0 + 4\mu_0} \mathbb{J} + \frac{3}{5\mu_0} \frac{\kappa_0 + 2\mu_0}{3\kappa_0 + 4\mu_0} \mathbb{K} \]  \hspace{1cm} (A.46)
A.3.2 Mori-Tanaka and Self Consistent estimates

Eshelby’s isolated inclusion solution can be used in order to generate estimates for the stiffness of a composite material.

The idea is the following: let us first consider that our composite is made of a main phase that plays the role of a matrix, with stiffness tensor $C_0$, and a few spherical inclusions of $N$ different materials, randomly distributed and with a stiffness tensor $C_i$, $i \in \{1, ..., N\}$. Further assume that the concentration $\phi_i$ of the inclusions is very small (dilute), in such a way that the inclusions are well separated from each other. Then it may be expected that the inclusions will not interact with each other and that the Eshelby’s result will be applicable. Therefore, the mean strain concentration tensor in each inclusion of phase $i$ will be:

$$\langle A_i(x) \rangle_{\Omega_i} = (I + P_0 : (C_i - C_0))^{-1}$$ \hspace{1cm} (A.47)

Now, as the concentration of inclusions increases, the influence of the interactions will become non negligible and the strain field inside the inclusions will deviate from the Eshelby’s solution. To take it into account, we consider that instead of being subjected to a strain $E$ at its boundary, the RVE is subjected to an auxiliary strain $\tilde{E}$, called screening field:

$$\langle \varepsilon (x) \rangle_{\Omega} = (I + P_0 : (C_i - C_0))^{-1} : \tilde{E}$$ \hspace{1cm} (A.48)

This screening field is determined by enforcing the relation $\langle \varepsilon (x) \rangle_{\Omega} = E$:

$$\sum_{i=0}^{N} \phi_i (I + P_0 : (C_i - C_0))^{-1} : \tilde{E} = E$$ \hspace{1cm} (A.49)

$$\Rightarrow \quad \tilde{E} = \left[ \sum_{i=0}^{N} \phi_i (I + P_0 : (C_i - C_0))^{-1} \right]^{-1} : E$$ \hspace{1cm} (A.50)

which we can rewrite

$$\tilde{E} = \left[ \sum_{i=0}^{N} \phi_i \tilde{A}_i \right]^{-1} : E$$ \hspace{1cm} (A.51)

with

$$\tilde{A}_i = (I + P_0 : (C_i - C_0))^{-1}$$ \hspace{1cm} (A.52)
Therefore, the mean strain can be expressed by:

\[
\langle \varepsilon(x) \rangle_{\Omega_i} = \bar{\varepsilon}_i : \bar{E} = \bar{\varepsilon}_i : \left[ \sum_{i=0}^{N} \phi_i \bar{A}_i \right]^{-1}
\]  
(A.53)

and the mean strain concentration tensor:

\[
\langle \Lambda(x) \rangle_{\Omega_i} = \bar{\Lambda}_i : \left[ \sum_{i=0}^{N} \phi_i \bar{A}_i \right]^{-1}
\]  
(A.54)

Finally, we reach an estimate for the homogeneous stiffness:

\[
C_{\text{hom}} = \sum_{i=0}^{N} \phi_i C_i : \langle \Lambda(x) \rangle_{\Omega_i}
\]  
(A.55)

\[
= \left[ \sum_{i=0}^{N} \phi_i C_i : \bar{\Lambda}_i \right] : \left[ \sum_{i=0}^{N} \phi_i \bar{A}_i \right]^{-1}
\]

It is interesting to note that this formula does not depend neither on the size of the inclusions nor on their positions. The only morphological information is introduced by the volume fractions \(\phi_i\). This property is very useful since it means that we don’t need to introduce any modelling of the position of each inclusion in order to get a good estimate.

**Remark 7** For clarity purposes, the derivation of formula (A.55) has been made considering spherical inclusions but it can be extended to any ellipsoidal shape provided that every inclusion of a same phase has the same shape.

Two schemes make use of relation (A.55) to generate estimates: the Mori Tanaka scheme and the Self Consistent scheme. The difference between these two lies in the choice of the reference stiffness \(C_0\).

**Mori Tanaka estimates**

The Mori Tanaka scheme confers to one phase the status of reference phase. It gives very good estimates when the composite has a clear Matrix - Inclusions morphology such as the one sketched in Fig A-3.
Figure A-3: Matrix-Inclusions morphology

In this case, we take the stiffness of the matrix phase as reference stiffness. Here are useful expressions obtained for a few particular cases. We assume that each phase have a isotropic behavior:

\[ C_i = 3\kappa_i J + 2\mu_i K \]  \hspace{2cm} (A.56)

**Solid + Voids**  This is the case of a porous material. The reference phase is the solid (\(\kappa_0 = \kappa_S, \mu_0 = \mu_S, \phi_0 = \phi_S\)) and the inclusions are voids (\(\kappa_1 = 0, \mu_1 = 0, \phi_1 = \phi_V\)). We obtain:

\[ \kappa_{\text{hom}} = \frac{4(1 - \phi_V)\kappa_S \mu_S}{3\phi_V \kappa_S + 4\mu_S} \]  \hspace{2cm} (A.57)
\[ \mu_{\text{hom}} = \frac{(1 - \phi_V)(9\kappa_S + 8\mu_S)\mu_S}{(6\phi_V + 9)\kappa_S + (12\phi_V + 8)\mu_S} \]

**Solid + Rigid inclusions with perfect adhesion**  The reference phase is the solid (\(\kappa_0 = \kappa_S, \mu_0 = \mu_S, \phi_0 = \phi_S\)) and the inclusions are rigid inclusions (\(\kappa_1 = \infty, \mu_1 = \infty, \phi_1 = \phi_R\)). We obtain:

\[ \kappa_{\text{hom}} = \frac{13\kappa_S + 4\phi_R\mu_S}{3 \left(1 - \phi_R\right)} \]  \hspace{2cm} (A.58)
\[ \mu_{\text{hom}} = \frac{1((9\phi_R + 6)\kappa_S + (8\phi_R + 12)\mu_S)\mu_S}{4 \left(1 - \phi_R\right) \left(2\mu_S + \kappa_S\right)} \]
Solid + Rigid inclusions with slippery imperfect interfaces  The derivation of this case is different. Indeed, Eshelby problem was assuming a perfect adhesion at the interface of the two materials so we cannot use this result. R.M. Christensen and K.H. Lo have adapted Eshelby’s problem to the case of a rigid inclusion with slippery imperfect interface [24] [5]. The result is the following:

\[
\frac{1}{|\mathcal{O}|} \int_{\partial \mathcal{O}} \frac{1}{2} (\{\xi\} \otimes n + n \otimes \{\xi\}) \ d\tau = \left[ \frac{3\kappa_0 + 4\mu_0}{5\kappa_0 + 8\mu_0} \right] : \mathbf{E}^\infty
\]

\[
\frac{1}{|\mathcal{O}|} \int_{\partial \mathcal{O}} \mathbf{x} \otimes \sigma(\mathbf{x}) \cdot n \ dS = \left[ \frac{3\kappa_0 + 4\mu_0}{5\kappa_0 + 8\mu_0} \right] : \mathbf{E}^\infty
\]

Then, applying the same reasoning as before, the Mori Tanaka estimate reads:

\[
\kappa_{\text{hom}} = \frac{1}{3} \left( \frac{3\kappa_S + 4\phi_L \mu_S}{1 - \phi_L} \right)
\]

\[
\mu_{\text{hom}} = \frac{1}{3} \frac{\mu_S ((9\phi_L + 15) \kappa_S + (8\phi_L + 24) \mu_S)}{(5 - 2\phi_L) \kappa_S + (8 - 4\phi_L) \mu_S}
\]

where \( \phi_L \) is the volume fraction of inclusions.

Self consistent estimates

Although in some cases it is possible to identify a main phase that plays a clear role of matrix, this is not always the case. The Self Consistent scheme is based on the idea that we cannot choose one particular phase as the reference one. It is especially suitable for disordered materials such as the one sketched in Fig A-4.

We choose as reference stiffness the homogeneous stiffness which means that we have to solve for \( C_{\text{hom}} \) in the following equation:

\[
C_{\text{hom}} = \left[ \sum_{i=0}^{N} \phi_i \mathbf{C}_i : \left( I + P_0 : \left( \mathbf{C}_i - C_{\text{hom}} \right) \right)^{-1} \right] : \left[ \sum_{i=0}^{N} \phi_i \left( I + P_0 : \left( C_i - C_{\text{hom}} \right) \right)^{-1} \right]^{-1}
\]

Solid + Voids  In the case of a porous material, we observe an interesting feature of the self consistent scheme which is that equation (A.61) does not have any reasonable (positive) solution for a porosity greater than 0.5. This is interpreted as the translation of the percolation
Figure A-4: Disordered morphology

phenomenon in which the solid looses its mechanical performances below a certain packing density.

The values of the homogeneous stiffness are \((\phi_V \leq \frac{1}{2})\):

\[
\kappa_{\text{hom}} = \frac{1}{29} \phi_V \kappa_S + \frac{\kappa_S}{12 - 20 \phi_V} \mu_S (3 \phi_V (3 - \phi_V) \kappa_S + (24 + 20 \phi_V^2 - 56 \phi_V) \mu_S \\
... - \phi_V \sqrt{81 \kappa_S^2 - 168 \phi_V \kappa_S \mu_S - 54 \kappa_S^2 \phi_V + 144 \mu_S \kappa_S + 400 \phi_V^2 \mu_S^2} \\
... - 120 \kappa_S \phi_V^2 \mu_S - 320 \phi_V \mu_S^2 + 9 \kappa_S^2 \phi_V^2 + 64 \mu_S^2 \tag{A.62}
\]

\[
\mu_{\text{hom}} = \frac{1}{16} ((8 - 20 \phi_V) \mu_S + (3 \phi_V - 9) \kappa_S \\
... + \sqrt{81 \kappa_S^2 - 168 \phi_V \kappa_S \mu_S - 54 \kappa_S^2 \phi_V + 144 \mu_S \kappa_S + 400 \phi_V^2 \mu_S^2} \\
... - 120 \kappa_S \phi_V^2 \mu_S - 320 \phi_V \mu_S^2 + 9 \kappa_S^2 \phi_V^2 + 64 \mu_S^2 \tag{A.63}
\]

**Solid + Rigid inclusions with perfect adhesion** In this case also, the volume fraction of rigid inclusions has to be less than \(\frac{1}{2}\):

\[
\kappa_{\text{hom}} = \frac{1}{18 (1 - \phi_R) (1 - 2 \phi_R)} ((18 + 15 \phi_R^2 - 42 \phi_R) \kappa_S + 4 \phi_R (3 - \phi_R) \mu_S \\
... + \phi_R \sqrt{16 \phi_R^2 \mu_S^2 - 168 \phi_R \mu_S \kappa_S - 120 \phi_R^2 \mu_S \kappa_S - 56 \phi_R \mu_S \kappa_S^2 - 36 \kappa_S^2} \\
... - 180 \kappa_S^2 \phi_R + 144 \mu_S \kappa_S + 225 \kappa_S^2 \phi_R^2 + 144 \mu_S^2 \tag{A.64}
\]

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\[
\mu_{\text{hom}} = \frac{1}{24} \frac{1}{1 - 2 \phi_R} \left( (15 \phi_R - 6) \kappa_S + (12 - 4 \phi_R) \mu_S \right.
\]
\[
+ \sqrt{16 \phi_R^2 \mu_S^2 - 168 \phi_R \mu_S \kappa_S - 120 \phi_R^2 \mu_S \kappa_S - 96 \phi_R \mu_S^2 + 36 \kappa_S^2}
\]
\[
\left. - 180 \kappa_S^2 \phi_R + 144 \mu_S \kappa_S + 225 \kappa_S^2 \phi_R^2 + 144 \mu_S^2 \right)
\]
(A.65)

**Solid + Rigid inclusions with slippery imperfect interfaces**  As in the case of the Mori Tanaka scheme, we must adapt the procedure. We obtain the following homogeneous stiffness coefficients with a limitation on the volume fraction of inclusion, \( \phi_L \leq \frac{2}{3} 
\]

\[
\kappa_{\text{hom}} = \frac{1}{18} \frac{1}{(1 - \phi_L)(2 - 3 \phi_L)} \left( (3 (8 \phi_L^2 - 23 \phi_L + 12)) \kappa_S + 8 \phi_L (3 - 2 \phi_L) \mu_S \right.
\]
\[
+ \phi_L \sqrt{225 \kappa_S^2 + 720 \mu_S \kappa_S - 1392 \kappa_S \mu_S \phi_L - 720 \kappa_S^2 \phi_L + 576 \mu_S^2}
\]
\[
\left. - 768 \mu_S^2 \phi_L + 256 \mu_S^2 \phi_L^2 + 528 \mu_S \phi_L^2 \kappa_S + 576 \kappa_S^2 \phi_L^2 \right)
\]
(A.66)

\[
\mu_{\text{hom}} = \frac{1}{24} \frac{1}{2 - 3 \phi_L} \left( (24 - 16 \phi_L) \mu_S - (15 - 24 \phi_L) \kappa_S \right.
\]
\[
+ \sqrt{225 \kappa_S^2 + 720 \mu_S \kappa_S - 1392 \kappa_S \mu_S \phi_L - 720 \kappa_S^2 \phi_L + 576 \mu_S^2}
\]
\[
\left. - 768 \mu_S^2 \phi_L + 256 \mu_S^2 \phi_L^2 + 528 \mu_S \phi_L^2 \kappa_S + 576 \kappa_S^2 \phi_L^2 \right)
\]
(A.67)

### A.4 Variational formulation

A variational approach turns out to be very suitable for the study of composite materials, particularly in the presence of a non linear behavior. It allows the determination of bounds as well as a quantification of the accuracy of an approximate solution to the problem.

#### A.4.1 Integral equation formulation

Whether we consider a linear or a non-linear material, it is possible to characterize its behavior by a strain energy density function \( \omega (\varepsilon, \varepsilon) \). The constitutive relation linking the stress to the strain classically reads:

\[
\sigma = \frac{\partial \omega}{\partial \varepsilon} = \frac{\partial \omega}{\partial \varepsilon_{ji}} \varepsilon_i \otimes \varepsilon_j
\]
(A.68)

It is assumed that \( \omega \) is a convex function of the infinitesimal strain \( \varepsilon \). In the case of elasticity, we the strain energy density function is expressed by: \( \omega (\varepsilon) = \frac{1}{2} \varepsilon : \mathbf{C} : \varepsilon \). In addition, if we
introduce the potential energy functional:

\[ \Psi (\xi^*(x)) = \int_{\Omega} \omega (x, \varepsilon (\xi^*)) \, dx - \int_{\Omega} \mathbf{f} \cdot \xi^* \, dx - \int_{\partial\Omega} T^d \xi^*_i \, dS \]  

(A.69)

then it can be shown, [87], that the displacement field \( \xi (x) \) solution to the problem minimizes \( \Psi \) over the set of "trial" kinematically admissible displacement fields:

\[ \Psi (\xi (x)) = \min_{\xi \in \mathcal{K}} \Psi (\xi^*(x)) \]  

(A.70)

with \( \mathcal{K} = \{ \xi^* (x), \xi^* (x) = \xi_0 (x) \text{ on } \partial\Omega_{\xi^0} \} \)

where \( \xi_0 \) is the prescribed displacement field on the boundary. This variational formulation is a classical result of continuum mechanics and is, for instance, the basis of the Finite Element Method. Now if we specialize equation (A.69) to the case of problem (A.21) posed with displacement boundary conditions, we obtain:

\[ \Psi (\xi^*(x)) = \int_{\Omega} \omega (x, \varepsilon (\xi^*)) \, dx \]  

(A.71)

and the set of kinematically admissible fields becomes:

\[ \mathcal{K} (E) = \{ \xi^* (x), \xi^* (x) = E \cdot x \text{ on } \partial\Omega \} \]  

(A.72)

The solution to problem (A.21) minimizes \( \Psi \) so dividing by the volume of the RVE, we can define the macroscopic strain energy function:

\[ \mathcal{W} (E) = \frac{1}{|\Omega|} \min_{\xi^* \in \mathcal{K}(E)} \int_{\Omega} \omega (x, \varepsilon (\xi^*)) \, dx = \min_{\xi^* \in \mathcal{K}(E)} \langle \omega (x, \varepsilon (\xi^*)) \rangle \]  

(A.73)

It is possible to demonstrate, [84], that we have a similar type of relation for the macroscopic quantities as for the microscopic ones (Eq. A.68):

\[ \Sigma = \frac{\partial \mathcal{W}}{\partial E} \]  

(A.74)
Dual formulation

Similarly, it is possible to introduce the complementary energy density function, $u$, defined as the Legendre transformation of $\omega$:

$$u(x, \sigma) = \omega^*(x, \sigma) := \sup_{\varepsilon} \{ \sigma : \varepsilon - \omega(x, \varepsilon) \} \quad (A.75)$$

Then we have the dual property:

$$\varepsilon = \frac{\partial u}{\partial \sigma} \quad (A.76)$$

Now, introducing the complementary energy functional, $V$, and specializing it to the case of problem (A.21) posed with loading boundary conditions, we obtain:

$$\mathcal{U}(\Sigma) = \frac{1}{|\Omega|} \min_{\sigma^* \in \mathcal{S}(\Sigma)} \int u(x, \sigma^*(x)) \, dx = \min_{\sigma^* \in \mathcal{S}(\Sigma)} (u(x, \sigma^*(x))) \quad (A.77)$$

with

$$\mathcal{S}(\Sigma) = \{ \sigma^*(x), \text{div} (\sigma^*(x)) = 0 \text{ in } \Omega \text{ and } \sigma^*(x) \cdot n = \Sigma \cdot n \text{ on } \partial \Omega \}$$

and the macroscopic constitutive relation reads:

$$E = \frac{\partial \mathcal{U}}{\partial \Sigma} \quad (A.78)$$

A.4.2 Voigt and Reuss Bounds

This variational formulation can be used to generate rigorous bounds for the homogeneous stiffness of a composite material. The well known Voigt and Reuss bounds can be easily derived from equations (A.73) and (A.77). Indeed, the simplest trial fields we can think of are the unperturbed fields, namely:

$$\xi^*(x) = E \cdot x \quad \Rightarrow \quad \varepsilon^*(x) = E \quad (A.79)$$

for the first equation, and

$$\sigma^*(x) = \Sigma \quad (A.80)$$

for the second. Since in the case of elasticity, the expression of $\omega$ and $u$ are $\omega(\varepsilon) = \frac{1}{2} \varepsilon : C : \varepsilon$ and $u(\sigma) = \frac{1}{2} \sigma : C^{-1} : \sigma$, and the one of $\mathcal{W}$ and $\mathcal{U}$ are $\mathcal{W}(E) = \frac{1}{2} E : C^{\text{hom}} : E$ and
\[ U(\Sigma) = \frac{1}{2} \Sigma : (C^{\text{hom}})^{-1} : \Sigma, \text{equation (A.73) gives us, for any } E: \]
\[ \frac{1}{2} E : C^{\text{hom}} : E \leq \left\langle \frac{1}{2} E : C(x) : E \right\rangle \]  \hspace{1cm} \text{(Voigt)} \tag{A.81}

and equation (A.77), for any \( \Sigma: \)
\[ \frac{1}{2} \Sigma : (C^{\text{hom}})^{-1} : \Sigma \leq \left\langle \frac{1}{2} \Sigma : C^{-1}(x) : \Sigma \right\rangle \]  \hspace{1cm} \text{(Reuss)} \tag{A.82}

That leads to the following inequalities:
\[ \left\langle \kappa(x)^{-1} \right\rangle^{-1} \leq \kappa^{\text{hom}} \leq \left\langle \kappa(x) \right\rangle \]  \hspace{1cm} \text{(A.83a)}
\[ \left\langle \mu(x)^{-1} \right\rangle^{-1} \leq \mu^{\text{hom}} \leq \left\langle \mu(x) \right\rangle \]  \hspace{1cm} \text{(A.83b)}

### A.4.3 Use of the Green function

It is possible to reach tighter bounds than the Voigt and Reuss bounds by resorting to the Green's function. Let us consider a "reference medium" occupying the same volume as the RVE but with constant elasticity tensor \( C_0 \). The polarization \( \tau \) is defined by:
\[ \tau = (C(x) - C_0) : \epsilon = \sigma - C_0 : \epsilon \]  \hspace{1cm} \text{(A.84)}

The principle of the procedure is the following:

1. At first, consider the polarization as already known.
2. Solve the problem with \( \tau \) being a parameter of the problem. Express the solution as a function of \( \tau \) (i.e. \( \epsilon = \epsilon(\tau) \)).
3. The actual value of \( \tau \) is the solution to the implicit equation:
   \[ \tau = (C(x) - C_0) : \epsilon(\tau) \]  \hspace{1cm} \text{(A.85)}
4. Finally, the actual polarization having been found, the solution to the problem is given
The introduction of the polarization in problem (A.21) transforms it into:

\[ \text{find } \xi(x) \text{ such that} \begin{cases} \text{div} \left( \mathbf{C}_0 : \frac{1}{2} \left( \text{grad } \xi + \tau \text{'grad } \xi \right) \right) + \text{div} (\tau) = 0 \quad \text{in } \Omega \\ \xi = \mathbf{E} \cdot \mathbf{x} \quad \text{on } \partial \Omega \end{cases} \] (A.87)

which we break down into two sub-problems:

**Problem 1:**

Find \( \xi_0(x) \) such that

\[ \begin{cases} \text{div} \left( \mathbf{C}_0 : \frac{1}{2} \left( \text{grad } \xi_0 + \tau \text{'grad } \xi_0 \right) \right) = 0 \quad \text{in } \Omega \\ \xi_0 = \mathbf{E} \cdot \mathbf{x} \quad \text{on } \partial \Omega \end{cases} \] (A.88)

**Problem 2:**

Find \( \xi'(x) \) such that

\[ \begin{cases} \text{div} \left( \mathbf{C}_0 : \frac{1}{2} \left( \text{grad } \xi' + \tau \text{'grad } \xi' \right) \right) + \text{div} (\tau) = 0 \quad \text{in } \Omega \\ \xi' = 0 \quad \text{on } \partial \Omega \end{cases} \] (A.89)

The resolution of Problem 1 is trivial: \( \xi_0(x) = \mathbf{E} \cdot \mathbf{x} \). However, Problem 2 is much more complex and requires the introduction of the corresponding Green function. Green's functions in general are functions used to solve non-homogeneous differential equations subject to boundary conditions. They are widely employed in many fields of physics. The idea is to define a Green's function \( G \) as a solution to \( \mathcal{D}G = \delta \), where \( \mathcal{D} \) is a differential operator and \( \delta \) is the Dirac distribution. By doing so, we can subsequently express any solution to the differential equation \( \mathcal{D}\varphi = f \) with the help of the Green's function: \( \varphi(x) = (G * f)(x) = \int G(x-y) f(y) \, dy \).

Because of its non-uniqueness, particular attention must be paid to the boundary conditions of the differential problem in the choice of the right Green function.

The use of such functions is quite complex and the complete derivation of the results is mathematically involved. Therefore, in this part, we will only summarize the main steps. The
derivation is inspired of [84]. The Green function associated with Problem 2 is defined by:

\[
\frac{\partial}{\partial x_j} \left[ C_{0_{ijkl}} \frac{\partial G_{kp}}{\partial x_l} (\mathbf{x}, \mathbf{x}') \right] + \delta_{ip} \delta (\mathbf{x} - \mathbf{x}') = 0 \quad \text{in } \Omega \tag{A.90}
\]

\[
G_{ip} (\mathbf{x}, \mathbf{x}') = 0 \quad \text{on } \partial \Omega
\]

And we can show that we can use it to express the solution of the problem as being:

\[
\xi_i (\mathbf{x}) = -\int_\Omega \frac{\partial G_{ip}}{\partial x_q} (\mathbf{x}, \mathbf{x}') \tau_{pq} (\mathbf{x}') \, d\mathbf{x}' \tag{A.91}
\]

and the corresponding strain:

\[
\varepsilon' (\mathbf{x}) = -\int_\Omega \Gamma (\mathbf{x}, \mathbf{x}') : \tau (\mathbf{x}') \, d\mathbf{x}' = - (\Gamma \times \tau) (\mathbf{x}) \tag{A.92a}
\]

with

\[
\Gamma_{ijkl} = \frac{1}{4} \left[ \frac{\partial^2 G_{ip}}{\partial x_j \partial x_k'} + \frac{\partial^2 G_{jp}}{\partial x_i \partial x_k'} + \frac{\partial^2 G_{iq}}{\partial x_j \partial x_p'} + \frac{\partial^2 G_{jq}}{\partial x_i \partial x_p'} \right] \tag{A.92b}
\]

The whole question is then to be able to get an explicit expression for the Green function. To do so, we make the assumption that the RVE is much larger than the size of the heterogeneities such that we can consider it as infinite. Then, by translation invariance, we can write the infinite-body Green function as a function of just one variable:

\[
G_\infty (\mathbf{x}, \mathbf{x}') = G_\infty (\mathbf{x} - \mathbf{x}', 0) \tag{A.93}
\]

Subsequently, use is made of the following wave plane decomposition of the three dimensional delta function:

\[
\delta (\mathbf{x}) = -\frac{1}{8\pi^2} \int_{||\mathbf{x}||=1} \delta'' (\mathbf{y} \cdot \mathbf{x}) \, dS \tag{A.94}
\]

which allows to reach the following integral expression for the Green function:

\[
G_\infty (\mathbf{x}) = \frac{1}{8\pi^2} \int_{||\mathbf{x}||=1} K (\mathbf{y})^{-1} \delta (\mathbf{y} \cdot \mathbf{x}) \, dS \tag{A.95a}
\]

with

\[
K_{ik} (\mathbf{y}) = C_{0_{ijkl}} v_j v_l \tag{A.95b}
\]

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and for the operator $\Gamma$:

$$
\Gamma_\infty (x) = -\frac{1}{8\pi^2} \int_{|\omega|=1} H(\omega) \delta''(\omega \cdot x) \, dS \tag{A.96a}
$$

with

$$
H_{ijpq} (\omega) = \left[ K(\omega)^{-1} \right]_{ij} v_j v_i \tag{A.96b}
$$

where indices $(ij)(pq)$ indicate double symmetrization like in equation (A.92b).

The implicit equation for $\tau$ is therefore:

$$
(\mathbf{C}(x) - \mathbf{C}_0)^{-1} : \tau(x) + (\Gamma * \tau)(x) = \mathbf{E} \tag{A.97}
$$

where $*$ designate the convolution product (A.92a). This equation is also known as the Lippmann-Schwinger equation. The operator $\Gamma$ is a distribution that only depends on the reference stiffness $\mathbf{C}_0$.

However the dependency on the composite stiffness and microstructure is introduced by $\mathbf{C}(x)$. The solution to this equation for $\tau$ is finally used to generate the solution of the problem: $\mathbf{e}(x) = (\mathbf{C}(x) - \mathbf{C}_0)^{-1} : \tau(x)$.

One may argue that equation (A.97) does not look easier to solve than the original problem. Although it may be true, this equation can be solved analytically in some special cases such as the Eshelby's isolated inclusion problem. The use of Green function can also be used to develop numerical methods aiming at approximating the resolution of the Lippmann-Schwinger equation and relying on Fast Fourier Transform as shown in [73]. Finally, it can be used to generate improved bounds known as Hashin-Shtrikman bounds.

### A.4.4 Hashin-Shtrikman bounds

Hashin-Shtrikman bounds were introduced in 1962 [52]. They make use of the concept of polarization and of Green function. In the case of an isotropic material, and without more information than the volume fractions of phases, they are the best bounds possibly available since one can exhibit morphologies that saturate the bounds.

The derivation of these bounds is based on the variational formulation (A.73). Let's assume
that $C_0 > C(x)$. Then, making use of the fact that:

$$\inf_{\tau} \left( \frac{\tau}{\tau} : \left( (C(x) - C_0)^{-1} : \tau \right) \right) = \frac{1}{2} \varepsilon : C(x) : \varepsilon - \frac{1}{2} \varepsilon : C_0 : \varepsilon \quad (A.98)$$

the variational formulation becomes:

$$\mathcal{W}(E) = \frac{1}{|\Omega|} \min_{\xi \in \mathcal{K}(E)} \int_{\Omega} \left[ \inf_{\tau} \left( \frac{\tau}{\tau} : \left( (C(x) - C_0)^{-1} : \tau \right) \right) + \frac{1}{2} \varepsilon : C_0 : \varepsilon d\mathbf{x} \right] \quad (A.99)$$

Interchanging the order of the infima over $\xi$ and $\tau$ we obtain:

$$\mathcal{W}(E) = \frac{1}{|\Omega|} \inf_{\tau} \left[ \left( \min_{\xi \in \mathcal{K}(E)} \int_{\Omega} \tau : \varepsilon + \frac{1}{2} \varepsilon : C_0 : \varepsilon d\mathbf{x} \right) - \int_{\Omega} \frac{1}{2} \tau : \left( (C(x) - C_0)^{-1} : \tau \right) d\mathbf{x} \right] \quad (A.100)$$

However, because of relation $\tau = \sigma - C_0 : \varepsilon$ the minimization over $\xi$ in the last equation is exactly the variational formulation of problem (A.87), where the polarization is fixed. So at the optimum,

$$\min_{\xi \in \mathcal{K}(E)} \int_{\Omega} \tau : \varepsilon + \frac{1}{2} \varepsilon : C_0 : \varepsilon d\mathbf{x} = \int_{\Omega} \tau : (E + \varepsilon') + \frac{1}{2} (E + \varepsilon') : C_0 : (E + \varepsilon') d\mathbf{x} \quad (A.101)$$

The application of Hill’s lemma gives $\int_{\Omega} E : C_0 : \varepsilon' d\mathbf{x} = 0$ and $\int_{\Omega} \tau : \varepsilon + \frac{1}{2} \varepsilon' : C_0 : \varepsilon' d\mathbf{x} = \int_{\Omega} \frac{1}{2} \tau : \varepsilon' d\mathbf{x}$. Further use of relation (A.92a) yields:

$$\mathcal{W}(E) = \frac{1}{|\Omega|} \inf_{\tau} \left[ \int_{\Omega} \tau : E - \frac{1}{2} \tau : (\Gamma \star \tau) - \frac{1}{2} \tau : (C(x) - C_0)^{-1} : \tau d\mathbf{x} \right] + \frac{1}{2} E : C_0 : E \quad (A.102)$$

which we can rewrite:

$$\mathcal{W}(E) = \inf_{\tau} \mathcal{H}(\tau) + \frac{1}{2} E : C_0 : E \quad (A.103a)$$

with

$$\mathcal{H}(\tau) = \frac{1}{|\Omega|} \int_{\Omega} \tau : E - \frac{1}{2} \tau : (\Gamma \star \tau) - \frac{1}{2} \tau : (C(x) - C_0)^{-1} : \tau d\mathbf{x} \quad (A.103b)$$

where $\mathcal{H}$ is the Hashin-Shtrikman functional. If at first we had chosen a stiffness $C_0$ such that $C_0 < C(x)$, then we would have reached the same result but with a sup instead of the inf. We can note that the optimality condition in the last equation retrieves the Lippmann-Schwinger
As many variational formulation, the interest of shifting the optimality condition from a optimization over displacement fields to an optimization over polarization is that we don’t have any constraint in the choice of trial polarization fields that will approximate the solution. Indeed, we can choose piecewise constant polarization:

\[ \boldsymbol{\tau}(x) = \tau_i \text{ for } x \in \Omega_i \]  
(A.104)

Then, the optimality conditions yield an upper bound (or a lower bound if \( C_0 < C(\bar{z}) \)) of the form:

\[ W(E) < W^{HS}(E) = \frac{1}{2} E : C^{HS} : E \]  
(A.105)

where \( C^{HS} \) is of the form:

\[ C^{HS} = \sum_i \phi_i C_i : A_i^{HS} \]  
(A.106)

Then it is possible to show that, if the composite material we consider is isotropic and statistically random, the tensors \( A_i^{HS} \) are expressed by:

\[ A_i^{HS} = (I + \mathbb{P}_0 : (C_i - C_0))^{-1} \left[ \sum_{i=0}^{N} \phi_i (I + \mathbb{P}_0 : (C_i - C_0))^{-1} \right]^{-1} \]  
(A.107)

which is very similar to the estimates of the previous section (A.55). The upper bound is obtained by the Mori-Tanaka scheme if the stiffest material is used as the matrix phase. Similarly, the lower bound is obtained if the most compliant material is chosen as the matrix phase. In particular, a very widely used result is that in the case of a composite made of a solid phase and some voids, regardless of its morphology, the Mori-Tanaka estimates are upper bounds of the exact stiffness coefficients.

**Remark 8** It has also been shown that these bounds are the exact estimates of a particular type of composites called Composite Sphere Assemblage. This example shows that without more information on our random material, it is impossible to reduce the bounds since in that case, the CSA would violate the new bounds.
A.5 Macroscopic strain energy of a two phase composite

The goal of this part is to derive the expression of the macroscopic strain energy function, $\mathcal{W}_0$, in the presence of prestress. These results are used in Chapters 2 and 3. Indeed, as it is pointed out, we need to resort to prestresses in order to keep a Comparison Composite with positive definite stiffness tensor (i.e. $\kappa > 0$ and $\mu > 0$). For clarity purposes, we will employ the formulation in strain rates used in these chapters ($\varepsilon$ is replaced by $d$ and $E$ by $D$).

Although in the purely linear case, $\mathcal{W}_0$ is simply expressed by $\mathcal{W}_0(D) = \frac{1}{2}D : \mathsf{C}^{\text{hom}} : D$ (Eq. A.35), its expression in the presence of prestress (thermoelastic) is more complex. That motivates this separate study of the macroscopic strain energy.

The calculation in the case of a composite with more than two phases is a very complex problem (although we can get self consistent estimates as in [60]). As it allows analytical simplifications, we will consider the case of a two phases composite with the following constitutive relation:

$$\sigma = C_i : d + \tau_i$$  \hfill (A.108)

A.5.1 Levin's theory

Based on the previous assumption on the behavior of the composite, the macroscopic strain energy density function can be expressed by:

$$\mathcal{W}_0 = \left\langle \frac{1}{2}d : \mathsf{C} : d \right\rangle_{\Omega} + \left\langle \tau : d \right\rangle_{\Omega}$$  \hfill (A.109)

Because of the presence of prestresses, we cannot apply the result of linear elasticity. The following study is based on the work of Levin [62]. The original thermoelastic problem is:

$$\mathcal{P} : \begin{cases} 
\text{div}(\sigma) = 0 & \text{in } \Omega \\
\sigma = C_i : d + \tau_i & \text{in } \Omega_i \\
d = \frac{1}{2}(\text{grad} \, v + \text{grad} \, \bar{v}) & \text{in } \Omega \\
v = D \cdot \bar{x} & \text{on } \partial \Omega 
\end{cases}$$  \hfill (A.110)
We break it down into two sub-problems:

\[ \mathcal{P} = \mathcal{P}' + \mathcal{P}'' \]  

(A.111)

with

\[
\begin{align*}
\mathcal{P}' : & \quad \left\{ \begin{array}{ll}
\text{div} (\mathbf{\sigma}') = 0 & \text{in } \Omega \\
\mathbf{\sigma}' = C_i : \mathbf{d}' & \text{in } \Omega_i \\
\mathbf{d}' = \frac{1}{2} (\text{grad } \mathbf{v}' + \text{grad } \mathbf{v}') & \text{in } \Omega \\
\mathbf{v}' = \mathbf{D} \cdot \mathbf{x} & \text{on } \partial \Omega 
\end{array} \right. \\
\mathcal{P}'' : & \quad \left\{ \begin{array}{ll}
\text{div} (\mathbf{\sigma}'') = 0 & \text{in } \Omega \\
\mathbf{\sigma}'' = C_i : \mathbf{d}'' + \mathbf{\tau}_i & \text{in } \Omega_i \\
\mathbf{d}'' = \frac{1}{2} (\text{grad } \mathbf{v}'' + \text{grad } \mathbf{v}'') & \text{in } \Omega \\
\mathbf{v}'' = 0 & \text{on } \partial \Omega
\end{array} \right.
\]

(A.112)

Then, the solution fields \( \mathbf{\sigma}(\mathbf{x}) \) and \( \mathbf{d}(\mathbf{x}) \) are the superposition of the solutions of the two sub-problems:

\[
\begin{align*}
\mathbf{\sigma}(\mathbf{x}) &= \mathbf{\sigma}'(\mathbf{x}) + \mathbf{\sigma}''(\mathbf{x}) \\
\mathbf{d}(\mathbf{x}) &= \mathbf{d}'(\mathbf{x}) + \mathbf{d}''(\mathbf{x})
\end{align*}
\]

(A.113)

Let us write \( \langle \mathbf{\sigma}''(\mathbf{x}) \rangle_\Omega = \mathbf{T} \). Since \( \mathcal{P}' \) is the classical linear problem we have \( \langle \mathbf{\sigma}'(\mathbf{x}) \rangle_\Omega = C^{\text{hom}} : \mathbf{D} \). So:

\[
\mathbf{\Sigma} = C^{\text{hom}} : \mathbf{D} + \mathbf{T}
\]

(A.114)

Now, in order to compute \( \mathbf{T} \), let us study the average \( \langle \mathbf{\sigma}''(\mathbf{x}) : \mathbf{d}'(\mathbf{x}) \rangle_\Omega \), for any boundary condition \( \mathbf{D} \). First, since \( \text{div} (\mathbf{\sigma}'') = 0 \) we can apply Hill’s lemma to get:

\[
\langle \mathbf{\sigma}''(\mathbf{x}) : \mathbf{d}'(\mathbf{x}) \rangle_\Omega = \langle \mathbf{\sigma}'(\mathbf{x}) \rangle_\Omega : \langle \mathbf{d}'(\mathbf{x}) \rangle_\Omega = \mathbf{T} : \mathbf{D}
\]

(A.115)

Second, let us make use of the constitutive relation of problem \( \mathcal{P}'' \): \( \mathbf{\sigma}'' = C : \mathbf{d}'' + \mathbf{\tau} \).

\[
\langle \mathbf{\sigma}''(\mathbf{x}) : \mathbf{d}'(\mathbf{x}) \rangle_\Omega = \langle \mathbf{\sigma}'(\mathbf{x}) : C : \mathbf{d}'(\mathbf{x}) \rangle_\Omega + \langle \mathbf{\tau} : \mathbf{d}'(\mathbf{x}) \rangle_\Omega
\]

(A.116)

where we recognize \( C : \mathbf{d}'(\mathbf{x}) = \mathbf{\sigma}'(\mathbf{x}) \). Since \( \mathbf{\sigma}'(\mathbf{x}) \) is divergence free, we can apply Hill’s lemma to the first right term which cancels it. Finally, recalling that \( \mathcal{P}' \) is a classical linear
problem we have \( \mathbf{d}'(\mathbf{x}) = \mathbf{A}(\mathbf{x}) : \mathbf{D} \). So:

\[
\langle \sigma''(\mathbf{x}) : \mathbf{d}'(\mathbf{x}) \rangle_{\Omega} = \langle \tau : \mathbf{A}(\mathbf{x}) \rangle_{\Omega} : \mathbf{D} \tag{A.117}
\]

Comparing equation (A.115) to equation (A.117), we reach the following expression of \( T \):

\[
T = \langle \tau : \mathbf{A}(\mathbf{x}) \rangle_{\Omega} = \sum_{i} \phi_{i} \tau_{i} : \langle \mathbf{A}(\mathbf{x}) \rangle_{\Omega_{i}} \tag{A.118}
\]

This result is very profitable since it allows to deduce the macroscopic thermoelastic behavior from the study of the linear elastic case \( \langle \mathbf{A}(\mathbf{x}) \rangle_{\Omega_{i}} \).

Now, using the quantities of the two sub-problems in the expression of the macroscopic strain energy (A.109), we obtain:

\[
\mathcal{W}_{0} = \left\langle \frac{1}{2} \mathbf{d}' : \mathbf{C} : \mathbf{d}' \right\rangle_{\Omega} + \left\langle \frac{1}{2} \mathbf{d}'' : \mathbf{C} : \mathbf{d}'' \right\rangle_{\Omega} + \left\langle \mathbf{d}' : \mathbf{C} : \mathbf{d}'' \right\rangle_{\Omega} + \langle \tau : \mathbf{d}' \rangle_{\Omega} + \langle \tau : \mathbf{d}'' \rangle_{\Omega} \tag{A.119}
\]

Let us study each term in detail:

1. The first term is the energy of the linear composite: \( \left\langle \frac{1}{2} \mathbf{d}' : \mathbf{C} : \mathbf{d}' \right\rangle_{\Omega} = \frac{1}{2} \mathbf{D} : \mathbf{C}^{\text{hom}} : \mathbf{D} \).

2. The second term can be simplified using the constitutive relation of problem \( P'' \): \( \sigma'' = \mathbf{C} : \mathbf{d}'' + \tau \). Then we obtain that \( \left\langle \frac{1}{2} \mathbf{d}'' : \mathbf{C} : \mathbf{d}'' \right\rangle_{\Omega} = \left\langle \frac{1}{2} \sigma'' : \mathbf{d}'' \right\rangle_{\Omega} - \frac{1}{2} \langle \tau : \mathbf{d}'' \rangle_{\Omega} \). Because of Hill's lemma, the first term in last expression in zero such that: \( \left\langle \frac{1}{2} \mathbf{d}'' : \mathbf{C} : \mathbf{d}'' \right\rangle_{\Omega} = -\frac{1}{2} \langle \tau : \mathbf{d}'' \rangle_{\Omega} \).

3. Noting that \( \mathbf{C} : \mathbf{d}'(\mathbf{x}) = \sigma'(\mathbf{x}) \), we can apply Hill's lemma to the third and show that it is zero.

4. Finally, as proved by relation (A.116), \( \langle \tau : \mathbf{d}'(\mathbf{x}) \rangle_{\Omega} = \mathbf{T} : \mathbf{D} \).

As a consequence, expression (A.119) can be rewritten in the form:

\[
\mathcal{W}_{0} = \frac{1}{2} \mathbf{D} : \mathbf{C}^{\text{hom}} : \mathbf{D} + \mathbf{T} : \mathbf{D} + \frac{1}{2} \langle \tau : \mathbf{d}'' \rangle_{\Omega} = \frac{1}{2} \mathbf{D} : \mathbf{C}^{\text{hom}} : \mathbf{D} + \mathbf{T} : \mathbf{D} + \sum_{i} \phi_{i} \tau_{i} : \langle \mathbf{d}'' \rangle_{\Omega_{i}} \tag{A.120}
\]
This last relation will be used to generate explicit expressions for \( \mathcal{W}_0 \). For their practical application in Chapter 3, we want expressions in terms of \( C^{\text{hom}}, \tau, \) and \( D \). To do so, we need to know the expression of \( T \) (which involves the phase averages of the strain concentration tensors \( \langle A \rangle_{\Omega_i} \) and the one of the different \( \langle d'' \rangle_{\Omega_i} \)). This is the object of the next sub-section on field statistics.

### A.5.2 Field statistics

Let us start with the determination of \( T \). Expression (A.118) specialized for a two phase composite without discontinuities reads:

\[
T = \phi_1 \tau_1 : \langle A \rangle_{\Omega_1} + \phi_2 \tau_2 : \langle A \rangle_{\Omega_2} \tag{A.121}
\]

In order to compute the phase averages \( \langle A \rangle_{\Omega_1} \) and \( \langle A \rangle_{\Omega_2} \), we make use of the expression of \( C^{\text{hom}} \) and of the average of the strain concentration tensor:

\[
\begin{cases} 
C^{\text{hom}} = \phi_1 C_1 : \langle A \rangle_{\Omega_1} + \phi_2 C_2 : \langle A \rangle_{\Omega_2} \\
I = \phi_1 \langle A \rangle_{\Omega_1} + \phi_2 \langle A \rangle_{\Omega_2} 
\end{cases} \tag{A.122}
\]

We now realize the advantage of considering a two phases composite: we only have two equations but we are just looking for two unknowns. The resolution of this system reads:

\[
\begin{cases} 
\phi_1 \langle A \rangle_{\Omega_1} = (C_1 - C_2)^{-1} : (C^{\text{hom}} - C_2) \\
\phi_2 \langle A \rangle_{\Omega_2} = (C_2 - C_1)^{-1} : (C^{\text{hom}} - C_1)
\end{cases} \tag{A.123}
\]

So the final expression of \( T \) is:

\[
T = (\tau_1 - \tau_2) : (C_1 - C_2)^{-1} : (C^{\text{hom}} - C_2) + \tau_2 \tag{A.124}
\]

Now let us determine the phase averages of the strain rate in the second sub-problem \( P'' \).

We have two equation: the expression of the average of the strain rate and the one of the average of the stress. It should be emphasized that although some estimates of \( \langle A \rangle_{\Omega_4} \) could be obtained using specific linear schemes such as the Mori-Tanaka or the Self Consistent scheme,
the expression of the strain rate averages in $\mathcal{P}'$ would be much more complex to obtain [60]:

\[
\begin{align*}
\phi_1 (\mathbf{d}'' \mid \Omega_1) + \phi_2 (\mathbf{d}'' \mid \Omega_2) &= 0 \\
\phi_1 (\mathbf{C}_1 : (\mathbf{d}'' \mid \Omega_1 + \boldsymbol{\tau}_1)) + \phi_2 (\mathbf{C}_2 : (\mathbf{d}'' \mid \Omega_2 + \boldsymbol{\tau}_2)) &= \mathbf{T}
\end{align*}
\] (A.125)

We solve this 2 by 2 system:

\[
\begin{align*}
\phi_1 (\mathbf{d}'' \mid \Omega_1) &= (\mathbf{C}_1 - \mathbf{C}_2)^{-1} : (\mathbf{T} - \phi_1 \boldsymbol{\tau}_1 - \phi_2 \boldsymbol{\tau}_2) \\
\phi_2 (\mathbf{d}'' \mid \Omega_2) &= (\mathbf{C}_2 - \mathbf{C}_1)^{-1} : (\mathbf{T} - \phi_1 \boldsymbol{\tau}_1 - \phi_2 \boldsymbol{\tau}_2)
\end{align*}
\] (A.126)

Finally, the expression of the macroscopic strain energy density is:

\[
\begin{align*}
\mathcal{W}_0 &= \frac{1}{2} \mathbf{D} : \mathbf{C}^\text{hom} : \mathbf{D} + \left[ (\mathbf{C}_1 - \mathbf{C}_2)^{-1} : (\mathbf{C}^\text{hom}_1 - \mathbf{C}_1) + \mathbf{C}_2 \right] : \mathbf{D} \\
&\quad + \frac{1}{2} (\boldsymbol{\tau}_1 - \boldsymbol{\tau}_2) : \left( (\mathbf{C}_1 - \mathbf{C}_2)^{-1} : (\mathbf{C}^\text{hom}_1 - \mathbf{C}_2) - \phi_1 \mathbf{I} \right) : (\mathbf{C}_1 - \mathbf{C}_2)^{-1} : (\boldsymbol{\tau}_1 - \boldsymbol{\tau}_2)
\end{align*}
\] (A.127)

It should be emphasized that special care must be given to the order of the products. Indeed, even though these expressions involve only stiffness tensors, which have minor and major symmetry, the product of two stiffness tensors does not a priori have the major symmetry. However, in the case of isotropic tensors, since $\mathbf{J} : \mathbf{K} = \mathbf{K} : \mathbf{J} = 0$, they all commute so major symmetry is conserved.

Last expression can be simplified in special cases.

### A.5.3 Specialized expressions

We consider a case that will be useful in following developments of Chapter 3: only one phase has a prestress and this prestress is a pressure (no deviatoric component).

**Solid + Voids**

We set:

\[
\begin{align*}
\boldsymbol{\tau}_1 &= \tau_{1m} \mathbf{1} \\
\mathbf{C}_2 &= 0 \\
\boldsymbol{\tau}_2 &= 0
\end{align*}
\] (A.128)
Then,

\[ W_0 = \frac{1}{2} D : C^{\text{hom}} : D + \tau_1 : C^{-1} : C^{\text{hom}} : D + \frac{1}{2} \tau_1 : \left( C^{-1} : C^{\text{hom}} - \phi_1 I \right) : C^{-1} : \tau_1 \] (A.129)

\[ T = \tau_1 : C^{-1} : C^{\text{hom}} \]

\[ \Sigma = C^{\text{hom}} : D + T \]

which we can express in the isotropic case as:

\[ W_0 = \frac{1}{2} \kappa^{\text{hom}} D_v^2 + \mu^{\text{hom}} D_d^2 + \kappa^{\text{hom}} \tau_{1m} D_v + \frac{1}{2} \phi_1 \left( \frac{\kappa^{\text{hom}}}{\kappa_1} - \phi_1 \right) \tau_{1m}^2 \] (A.130)

with \( D_v = tr(D) \) and \( D_d = \sqrt{\Delta : \Delta} \) where \( \Delta = D - \frac{1}{3} tr(D) \). As we will need it in Chapter 3, the correspondence between the stress and strain quantities is:

\[ D_v = \frac{1}{\kappa^{\text{hom}}} \left( \Sigma_m - \frac{\kappa^{\text{hom}}}{\kappa_1} \tau_{1m} \right) \] (A.131)

\[ D_d = \frac{1}{2\mu^{\text{hom}}} \Sigma_d \]

**Solid + Rigid inclusions**

We set:

\[ \tau_1 = \tau_{1m} 1 \] (A.132)

\[ C_2 \to \infty \]

\[ \tau_2 = 0 \]

Then,

\[ W_0 = \frac{1}{2} D : C^{\text{hom}} : D + \tau_1 : D \] (A.133)

\[ T = \tau_1 \]

\[ \Sigma = C^{\text{hom}} : D + T \]
which we can express in the isotropic case as:

$$\mathcal{W}_0 = \frac{1}{2} \kappa^{\text{hom}} D_v^2 + \mu^{\text{hom}} D_d^2 + \tau_{1m} D_v$$  \hfill (A.134)

The correspondence between the stress and strain quantities is:

$$D_v = \frac{1}{\kappa^{\text{hom}}} (\Sigma_m - \tau_{1m})$$  \hfill (A.135)

$$D_d = \frac{1}{2\mu^{\text{hom}}} \Sigma_d$$

**A.5.4 Case with discontinuities**

The case with discontinuities is studied in reference to the imperfect interface model developed in Chapter 3. In order to obtain an estimate of $\mathcal{W}_0$, we must assume that:

- The discontinuities in displacement are tangent to the interface:
  $$[[z]] \perp \mathbf{n}$$  \hfill (A.136)

- There is no shear force transmitted by the weak interfaces (perfect slip):
  $$\mathbf{\sigma} \cdot \mathbf{n} \parallel \mathbf{n}$$  \hfill (A.137)

We also make the same assumptions as in the case with perfect adhesion (A.132):

$$\tau_1 = \tau_{1m} \mathbf{1}$$  \hfill (A.138)

$$C_2 \to \infty$$

$$\tau_2 = 0$$
We denote \( \{d\} \) the strain rate distribution defined outside of the discontinuities. The expression for the macroscopic strain energy corresponding to (A.119) reads in this case:

\[
W_0 = \left\langle \frac{1}{2} \{d'\} : C : \{d'\} \right\rangle_{\Omega} + \left\langle \frac{1}{2} \{d''\} : C : \{d''\} \right\rangle_{\Omega} + \langle \{d'\} : C : \{d''\} \rangle_{\Omega} \\
+ \langle \tau : \{d'\} \rangle_{\Omega} + \langle \tau : \{d''\} \rangle_{\Omega}
\]  \hspace{1cm} (A.139)

A study of the first three terms leads to the following expressions:

\[
\left\langle \frac{1}{2} \{d'\} : C : \{d'\} \right\rangle_{\Omega} = \frac{1}{2} D : C_{\text{hom}} : D - \frac{1}{|\Omega|} \int_{\Omega} n \cdot \sigma' \cdot [[u']] d\pi \hspace{1cm} (A.140)
\]
\[
\left\langle \frac{1}{2} \{d''\} : C : \{d''\} \right\rangle_{\Omega} = -\frac{1}{2|\Omega|} \int_{\Omega} n \cdot \sigma'' \cdot [[u'']] d\pi - \frac{1}{2} \langle \tau : \{d''\} \rangle_{\Omega}
\]
\[
\langle \{d'\} : C : \{d''\} \rangle_{\Omega} = -\frac{1}{|\Omega|} \int_{\Omega} n \cdot \sigma' \cdot [[u'']] d\pi
\]

But because of relations (A.136) and (A.137), all the surface integrals are zero and we obtain:

\[
W_0 = \frac{1}{2} D : C_{\text{hom}} : D + \langle \tau : \{d'\} \rangle_{\Omega} + \frac{1}{2} \langle \tau : \{d''\} \rangle_{\Omega}
\]

Let us first study the last term of the previous expression. With the assumptions (A.138), the velocity field \( u'' = 0 \) is solution to \( P_j \) (with \( \sigma'' = \tau_{1m} 1 \) everywhere). Therefore \( \langle \tau : \{d''\} \rangle_{\Omega} = 0 \).

Now, let us study the term \( \langle \tau : \{d'\} \rangle_{\Omega} \). Because of the infinite stiffness of the inclusions, we have:

\[
\langle \tau : \{d'\} \rangle_{\Omega} = \phi_1 \tau_1 : \langle \{d'\} \rangle_{\Omega_1} = \phi_1 \tau_{1m} 1 : \langle \{A\} \rangle_{\Omega_1} : D
\]

Then, using the identity \( \langle A \rangle_{\Omega} = \phi_1 \langle \{A\} \rangle_{\Omega_1} + \phi_1 \langle a(x) \rangle_{\Omega_1} + \phi_2 \langle \{A\} \rangle_{\Omega_2} + \phi_2 \langle a(x) \rangle_{\Omega_2} \), we can express the term \( \phi_1 1 : \langle \{A\} \rangle_{\Omega_1} : D \) as:

\[
\phi_1 1 : \langle \{A\} \rangle_{\Omega_1} : D = 1 : D - \phi_1 1 : \langle a(x) \rangle_{\Omega_1} : D - \phi_2 1 : \langle a(x) \rangle_{\Omega_2} : D
\]

but because of the assumption (A.136), the integrals on the surfaces of discontinuity,

\[
\int_{\Omega \cap \Omega} \frac{1}{2} \left( [[u']] \otimes n + n \otimes [[u']] \right) d\pi
\]

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are purely deviatoric such that:

\[ 1 : \langle a(x) \rangle_{\Omega_1} = 1 : \langle a(x) \rangle_{\Omega_2} = 0 \]

So we obtain:

\[ \langle \tau : \{d'\} \rangle_{\Omega} = \tau_{1m} D_v \]

and

\[ \mathcal{W}_0 = \frac{1}{2} D : C^{\text{hom}} : D + \tau_{1m} D_v \]

which is the same expression as in the case with perfect adhesion. We only need to take the estimates of $C^{\text{hom}}$ corresponding to the case of rigid inclusions with slippery imperfect interface given by relations (A.60), (A.66) and (A.67).
Appendix B

Homogeneous indentation modulus

The aim of this second appendix is to make use of the linear homogenization techniques presented in Appendix A in order to link the homogeneous indentation modulus to the elastic and morphological properties of the microscopic constituents. We only consider the isotropic case.

The indentation modulus for a homogeneous medium is expressed by:

\[ M = \frac{E}{1 - \nu^2} \quad (B.1) \]

This expression involves the Young’s modulus and the Poisson’s ratio. However, in order to use the same elastic quantities as in the first appendix, we can express it as a function of \( \kappa \) and \( \mu \). Indeed, since we have:

\[
\nu = \frac{1}{2} \frac{3\kappa - 2\mu}{3\kappa + \mu} \quad (B.2)
\]

\[
E = \frac{9\kappa \mu}{3\kappa + \mu}
\]

we can plug these expression and obtain the following expression for the indentation modulus:

\[ M = \frac{4\mu (3\kappa + \mu)}{3\kappa + 4\mu} \quad (B.3) \]

The homogeneous indentation modulus \( M^{\text{hom}} \) has the same expression but it involves ho-
mogeneous quantities:

\[ M_{\text{hom}} = \frac{4\mu_{\text{hom}} (3\kappa_{\text{hom}} + \mu_{\text{hom}})}{3\kappa_{\text{hom}} + 4\mu_{\text{hom}}} \]  

(B.4)

**B.1 Porous phase with Mori-Tanaka scheme**

We can make use of formula (A.57) to link the homogeneous indentation modulus to the solid phase elastic properties in the case of the porous paste and using a Mori-Tanaka scheme. Then we can express it as a function of the Young’s modulus and the Poisson’s ratio. The homogeneous strength modulus is proportional to the Young’s modulus. By setting \( E = 1 \) and for the following set of values of the Poisson’s ratio \( \nu = \{0.05, 0.15, 0.25, 0.35, 0.45\} \) we obtain the curves displayed in Fig. B-1.

Then, if we normalize these curves dividing them by their top value, we obtain very consistent shapes (Fig. B-2).
Figure B-2: Evolution of the homogeneous indentation modulus with the Poisson’s ratio. Mori-Tanaka scheme. Data normalized to 1.
Figure B-3: Evolution of the homogeneous indentation modulus with the Poisson’s ratio. Self-Consistent scheme.

**B.2 Porous phase with Self-consistent scheme**

If we lead a similar analysis using the Self-Consistent scheme (Eqs. A.62 and A.63), we obtain the curves displayed in Fig. B-3 for $E = 1$ and $\nu = \{0.05, 0.15, 0.25, 0.35, 0.45\}$.

Then, if we normalize these curves, we also obtain very consistent shapes (Fig. B-4).

The relation $M(\eta)$ is found to be quasi-linear. It is actually linear if we set $\nu = 0.2$. Since the widely reported value of the Poisson’s ratio for geomaterials is 0.23, we can just assume that the self consistent estimate of the homogeneous modulus simply reads:

$$M(\eta) = m_s (2\eta - 1)$$  \hspace{1cm} (B.5)
Figure B-4: Evolution of the homogeneous indentation modulus with the Poisson’s ratio. Self-Consistent scheme. Data normalized to 1.
Appendix C

N-phases strength homogenization – Self consistent estimates

The goal of this appendix is to show how we could extend the non-linear homogenization procedure introduced in Chapter 2 (see Table 2.2) to the case of an N-phases composite with finite strength.

The critical point in this procedure will be the estimation of the macroscopic strain energy, $\mathcal{W}_0(D)$, and the derivation with respect to $\mu_i$, $i \in \{1..N\}$. Indeed, two problems are faced:

1. If we consider an hyperbole or an ellipse with $S_0 \neq 0$, we must use a Comparison Composite with volumetric prestress to ensure a positive comparison bulk modulus, $\kappa$. Although expression (A.127) could be used for $N = 2$, it is very difficult to extend it for $N > 2$ (see Section A.5). Therefore, we will only consider centered elliptical strength criteria of the form:

$$f_i(\sigma) = \left( \frac{\sigma_m}{A_i} \right)^2 + \left( \frac{\sigma_d}{\sqrt{2}B_i} \right)^2 \leq 1 \quad (C.1)$$

In this case, optimality equation (2.69) reads:

$$\forall i \in \{1..N\}, \quad \frac{\partial \Pi^{\text{hom}}}{\partial \mu_i} = \left( \frac{A_i}{B_i} \right)^2 \frac{\partial \mathcal{W}_0}{\partial \kappa_i} + \frac{\partial \mathcal{W}_0}{\partial \mu_i} - \phi_i \frac{1}{2} \left( \frac{B_i}{\mu_i} \right)^2 = 0 \quad (C.2)$$

2. Based on the previous assumption, we don’t need any volumetric prestress in our Comparison Composite. Then, the expression of the macroscopic strain energy can be simplified
Because of relation (C.2), we must be able to express the homogeneous stiffness coefficients \( \kappa_{\text{hom}} \) and \( \mu_{\text{hom}} \) as well as their first order derivatives with respect to \( \mu_i, \ i \in \{1..N\} \). As we will see, this is quite straightforward if we use a Mori-Tanaka scheme but it needs some reformulation in order to use the Self-Consistent scheme.

### C.1 Expression of the stiffness coefficients

Following Equation (A.46), the tensor \( \mathbb{P}_0 \) reads in the isotropic case:

\[
\mathbb{P}_0 = \frac{1}{3\kappa_0 + 4\mu_0} \mathbb{J} + \frac{3}{5\mu_0} \kappa_0 + \frac{2\mu_0}{3\kappa_0 + 4\mu_0} \mathbb{K}
\]  

(C.4)

and the tensor \( \mathbb{A}_i \) reads for each phase (A.52):

\[
\mathbb{A}_i = (I + \mathbb{P}_0 : (\mathbb{C}_i - \mathbb{C}_0))^{-1}
\]  

\[
= \kappa_{\text{A}_i} \mathbb{J} + \mu_{\text{A}_i} \mathbb{K}
\]  

(C.5)

with

\[
\kappa_{\text{A}_i} = \frac{1}{3} \left( \frac{3\kappa_0 + 4\mu_0}{3\kappa_i + 4\mu_0} \right)
\]  

(C.6)

\[
\mu_{\text{A}_i} = \frac{5}{2} \frac{\mu_0 (3\kappa_0 + 4\mu_0)}{\mu_0 (9\kappa_0 + 8\mu_0) + 6\mu_1 (\kappa_0 + 2\mu_0)}
\]
C.1.1 Mori-Tanaka estimates

The stiffness coefficients of the homogeneous stiffness tensor obtained with the Mori-Tanaka scheme are (see Eq. (A.55)):

\[
\begin{align*}
\kappa^{\text{hom}} &= \frac{\sum_i \phi_i \kappa_i \kappa_{A_i}}{\sum_i \phi_i \kappa_{A_i}} \\
\mu^{\text{hom}} &= \frac{\sum_i \phi_i \mu_i \mu_{A_i}}{\sum_i \phi_i \mu_{A_i}}
\end{align*}
\]  

(C.7)

Contrary to the Self-Consistent scheme, these coefficients are explicit. Therefore, optimality equations (C.2) can be solved using numerical methods. As the focus of this appendix is on the use of the Self-Consistent scheme, we will not detail the procedure for the Mori-Tanaka scheme.

C.1.2 Self-Consistent estimates

In the case of the Self-Consistent scheme, the homogeneous coefficients are the solution to the system:

\[
\begin{align*}
\kappa^{\text{hom}} &= \kappa_0 = \frac{\sum_i \phi_i \kappa_i \kappa_{A_i}}{\sum_i \phi_i \kappa_{A_i}} \\
\mu^{\text{hom}} &= \mu_0 = \frac{\sum_i \phi_i \mu_i \mu_{A_i}}{\sum_i \phi_i \mu_{A_i}}
\end{align*}
\]  

(C.8a)

Replacing \( \kappa_{A_i} \) by expression (C.6), the first equation becomes:

\[
\kappa^{\text{hom}} = \kappa_0 = \frac{\sum_i \phi_i \frac{\kappa_i}{3\kappa_i + 4\mu_0}}{\sum_i \phi_i \frac{1}{3\kappa_i + 4\mu_0}}
\]  

(C.9)
in which we can make use of the property, $\kappa_i = \left(\frac{A_i}{B_i}\right)^2 \mu_i$:

$$\kappa^\text{hom} = \kappa_0 = \frac{\sum_i \phi_i \left(\frac{A_i}{B_i}\right)^2 \mu_i}{\sum_i \phi_i \left(\frac{A_i}{B_i}\right)^2 \mu_i + 4\mu_0}$$

(C.10)

so $\kappa^\text{hom} = \kappa_0$ is explicitly determined from the last equation as a function of $\mu^\text{hom} = \mu_0$ and of the comparison composite shear moduli of the different phases, $\mu_i, i \in \{1..N\}$:

$$\kappa^\text{hom} = \mathcal{F}(\mu^\text{hom}, \mu_i)$$

(C.11)

The real unknown of the problem is in fact $\mu^\text{hom} = \mu_0$. In general, after substitution $\kappa_i = \left(\frac{A_i}{B_i}\right)^2 \mu_i$, $\mu^\text{hom}$ is the result of a polynomial equation of degree $M$ ($M = 4$ for a 2 phases composite, $M = 13$ for a 3 phases composite, etc.):

$$\sum_{k=0}^{M} a_k (\mu^\text{hom})^k = 0$$

(C.12)

where the coefficients, $a_k$, are functions of $\mu_i, i \in \{1..N\}$.

A priori, such an equation cannot be solved analytically and therefore we cannot obtain analytical expressions of $\kappa^\text{hom}$ and $\mu^\text{hom}$ in order to differentiate them in the optimality equation (C.2). However, differentiating equation (C.12) with respect to $\mu_i$, we get:

$$\sum_{k=0}^{M} \frac{\partial a_k}{\partial \mu_i} (\mu^\text{hom})^k + \sum_{k=0}^{M} a_k k \frac{\partial (\mu^\text{hom})^k}{\partial \mu_i} (\mu^\text{hom})^{k-1} = 0$$

(C.13)
so the derivative \( \frac{\partial \mu_{\text{hom}}}{\partial \mu_i} \) can be expressed by:

\[
\frac{\partial \mu_{\text{hom}}}{\partial \mu_i} = \frac{\sum_{k=0}^{M} a_k (\mu_{\text{hom}})^k}{\sum_{k=0}^{M} a_k k (\mu_{\text{hom}})^{k-1}}
\]

Finally, making use of equation (C.11), we obtain for \( \kappa_{\text{hom}} \):

\[
\frac{\partial \kappa_{\text{hom}}}{\partial \mu_i} = \frac{\partial F}{\partial \mu_i} + \frac{\partial \mu_{\text{hom}}}{\partial \mu_i} \cdot \frac{\partial F}{\partial \mu_{\text{hom}}}
\]

### C.2 Numerical procedure

The interest of relations (C.14) and (C.15) is that we don’t need to obtain any analytical expressions for the homogeneous stiffness coefficients, \( \kappa_{\text{hom}} \) and \( \mu_{\text{hom}} \). We can leave \( \mu_{\text{hom}} \) as an unknown and just add (C.12) to the set of optimality equations. This section collects the equations of the problem and proposes a general procedure of resolution.

#### C.2.1 System of equations

Since in the previous developments, we have already replaced each occurrence of bulk moduli by their expressions in terms of shear moduli, \( \kappa_i = \left( \frac{A_i}{B_i} \right)^2 \mu_i \), we don’t have any derivative with respect to \( \kappa_i \) in the optimality equations. Equation (C.2) reads:

\[
\frac{1}{2} \frac{\partial \kappa_{\text{hom}}}{\partial \mu_i} D_v^2 + \frac{\partial \mu_{\text{hom}}}{\partial \mu_i} D_d^2 - \phi_i B_i^2 2\mu_i^2 = 0
\]

Then, replacing \( D_v \) and \( D_d \) by their expression in terms of the macroscopic stress invariants, \( \Sigma_m \) and \( \Sigma_d \), we obtain:

\[
\frac{1}{2} \frac{\partial \kappa_{\text{hom}}}{\partial \mu_i} \left( \frac{\Sigma_m}{\kappa_{\text{hom}}} \right)^2 + \frac{\partial \mu_{\text{hom}}}{\partial \mu_i} \left( \frac{\Sigma_d}{2\mu_{\text{hom}}} \right)^2 - \phi_i B_i^2 2\mu_i^2 = 0
\]
now, using (C.11) and (C.15), we have:

\[
\frac{1}{2} \left( \frac{\partial F}{\partial \mu^i} + \frac{\partial \mu^i_{\text{hom}}}{\partial \mu^i} \cdot \frac{\partial F}{\partial \mu^i_{\text{hom}}} \right) \left( \frac{\Sigma_m}{F(\mu^i_{\text{hom}}, \mu^i)} \right)^2 + \frac{\partial \mu^i_{\text{hom}}}{\partial \mu^i} \left( \frac{\Sigma_d}{2\mu^i_{\text{hom}}} \right)^2 - \phi_i \frac{B^2_i}{2\mu^2_i} = 0 \tag{C.18}
\]

or equivalently,

\[
\frac{1}{2} \frac{\partial F}{\partial \mu^i} \left( \frac{\Sigma_m}{F(\mu^i_{\text{hom}}, \mu^i)} \right)^2 + \left[ \frac{1}{2} \frac{\partial F}{\partial \mu^i_{\text{hom}}} \left( \frac{\Sigma_m}{F(\mu^i_{\text{hom}}, \mu^i)} \right)^2 + \left( \frac{\Sigma_d}{2\mu^i_{\text{hom}}} \right)^2 \right] \frac{\partial \mu^i_{\text{hom}}}{\partial \mu^i} = \phi_i \frac{B^2_i}{2\mu^2_i} \tag{C.19}
\]

To simplify the equations, we now introduce the following functions:

\[
G_i \left( \mu^i_{\text{hom}}, \mu^i \right) = \frac{\partial \mu^i_{\text{hom}}}{\partial \mu^i} = -\sum_{k=0}^{M} \frac{\partial a_k (\mu^i_{\text{hom}})^k}{\sum_{k=0}^{M} a_k k (\mu^i_{\text{hom}})^{k-1}} \tag{C.20}
\]

\[
H_i \left( \mu^i_{\text{hom}}, \mu^i, \Sigma_m \right) = \frac{1}{2} \frac{\partial F}{\partial \mu^i} \left( \frac{\Sigma_m}{F(\mu^i_{\text{hom}}, \mu^i)} \right)^2 \tag{C.21}
\]

\[
P \left( \mu^i_{\text{hom}}, \mu^i, \Sigma_m, \Sigma_d \right) = \frac{1}{2} \frac{\partial F}{\partial \mu^i_{\text{hom}}} \left( \frac{\Sigma_m}{F(\mu^i_{\text{hom}}, \mu^i)} \right)^2 + \left( \frac{\Sigma_d}{2\mu^i_{\text{hom}}} \right)^2 \tag{C.22}
\]

\[
Q \left( \mu^i_{\text{hom}}, \mu^i \right) = \sum_{k=0}^{M} a_k (\mu^i_{\text{hom}})^k \tag{C.23}
\]

Our system of equations becomes:

\[
P \left( \mu^i_{\text{hom}}, \mu^i, \Sigma_m, \Sigma_d \right) \cdot G_1 \left( \mu^i_{\text{hom}}, \mu^i \right) = \phi_1 \frac{B^2_1}{2\mu^2_1} - H_1 \left( \mu^i_{\text{hom}}, \mu^i, \Sigma_m \right) \tag{C.24}
\]

\[
P \left( \mu^i_{\text{hom}}, \mu^i, \Sigma_m, \Sigma_d \right) \cdot G_2 \left( \mu^i_{\text{hom}}, \mu^i \right) = \phi_2 \frac{B^2_2}{2\mu^2_2} - H_2 \left( \mu^i_{\text{hom}}, \mu^i, \Sigma_m \right) \tag{C.25}
\]

\[
\vdots
\]

\[
P \left( \mu^i_{\text{hom}}, \mu^i, \Sigma_m, \Sigma_d \right) \cdot G_N \left( \mu^i_{\text{hom}}, \mu^i \right) = \phi_N \frac{B^2_N}{2\mu^2_N} - H_N \left( \mu^i_{\text{hom}}, \mu^i, \Sigma_m \right) \tag{C.26}
\]

\[
Q \left( \mu^i_{\text{hom}}, \mu^i \right) = 0 \tag{C.27}
\]

Consequently, we obtain a system of \( N + 1 \) equations. We fix \( \Sigma_m \). Our unknowns are:

- \( \mu^i, i \in \{1..N\} \)
So we have \( N + 2 \) unknowns for \( N + 1 \) equations. The degree of freedom comes from the indetermination of yield design on the plastic multiplier, \( \lambda \), which here translates into an indetermination on a value of \( \mu_i \).

### C.2.2 Procedure of resolution

In order to solve our system of equations, we must resort to numerical techniques. When all the values of \( \mu_i, i \in \{1..N\} \) solution to the problem are strictly positive and finite, we can decrease the number of unknowns by decoupling the variable \( \Sigma_d \). Indeed, by dividing lines 2 to \( N \), we obtain the following system:

\[
\mathcal{P} (\mu^\text{hom}, \mu_i, \Sigma_m, \Sigma_d) \cdot \mathcal{G}_1 (\mu^\text{hom}, \mu_i) = \phi_1 \frac{B_1^2}{2\mu_1^4} - \mathcal{H}_1 (\mu^\text{hom}, \mu_i, \Sigma_m)
\]

\[
\mathcal{G}_2 (\mu^\text{hom}, \mu_i) \quad \frac{\mathcal{G}_1 (\mu^\text{hom}, \mu_i)}{\mathcal{G}_1 (\mu^\text{hom}, \mu_i)} = \frac{\phi_2 \frac{B_2^2}{2\mu_2^4} - \mathcal{H}_2 (\mu^\text{hom}, \mu_i, \Sigma_m)}{\phi_1 \frac{B_1^2}{2\mu_1^4} - \mathcal{H}_1 (\mu^\text{hom}, \mu_i, \Sigma_m)}
\]

\[
\vdots
\]

\[
\mathcal{G}_N (\mu^\text{hom}, \mu_i) \quad \frac{\mathcal{G}_1 (\mu^\text{hom}, \mu_i)}{\mathcal{G}_1 (\mu^\text{hom}, \mu_i)} = \frac{\phi_N \frac{B_N^2}{2\mu_N^4} - \mathcal{H}_N (\mu^\text{hom}, \mu_i, \Sigma_m)}{\phi_1 \frac{B_1^2}{2\mu_1^4} - \mathcal{H}_1 (\mu^\text{hom}, \mu_i, \Sigma_m)}
\]

\[
\mathcal{Q} (\mu^\text{hom}, \mu_i) = 0
\]

in which we can fix \( \mu_1 = 1 \), solve for \( \{\mu_i, i \in \{2..N\}, \mu^\text{hom}\} \) and then find the value of \( \Sigma_d \) from the first equation. However, this procedure of resolution assumes that all shear modulus are strictly positive and finite, which may not always be the case.
Homogeneous strength domain

Original strength domain

Solid + Voids estimate

Figure C-1: Convergence towards the case Solid + Voids. \([A_1 = 5; B_1 = 1; A_2 = 0.01; B_2 = 0.005; \phi_1 = 0.7; \phi_2 = 0.3]\)

C.3 Results for N=2

The method was tested in the case \(N = 2\). In order to validate the estimates obtained from this procedure, we tried to recover the two extreme cases that were derived analytically in Chapter 3: Solid + Voids (see Fig. C-1) and Solid + Rigid inclusions. (see Fig. C-2). In both cases, the estimates from this method converged towards the known solutions. However, as the values of the shear modulus became extreme (\(\mu_2 \to 0\) in the first case and \(\mu_1 \to \infty\) in the second case), some problems of convergence appeared and required some special attention.

In the case of Solid + Rigid inclusions, we found that the homogeneous strength domain converged towards the rigid case for a ratio between the strengths of the two materials of approximately 6 (or even less depending on the shapes of the ellipses). The interpretation of this result is that for such a ratio of strength properties, the second phase does not yield and behave as rigid inclusions.

As a short conclusion to this appendix, it appears that the method proposed for the strength homogenization of a N-phases composite can be implemented in practice and gives accurate results. Further work would be necessary in order to refine the numerical scheme for the resolution of the system of equations (C.21). However, the perspective of filling the gap between the two extreme cases, Solid + Voids and Solid + Rigid inclusions, and to get estimates for the
strength of highly heterogeneous material give it a clear interest.
Appendix D

Simulation data

This appendix gathers the simulation data obtained in Chapter 5.

It starts with the values of $H/c_s$ for the porous clay phase using the Mori-Tanaka scheme and the Self-Consistent scheme.

Then, at Level II, the choice of the scheme employed for the two homogenization steps and of the interfaces conditions lead to 8 different combinations (see Section 3.4.5).
Figure D-1: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level I - Mori-Tanaka scheme

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Figure D-2: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level I - Self-Consistent scheme

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Figure D-3: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level II - Mori-Tanaka + Mori-Tanaka - Perfectly adherent interfaces. [1/2]
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Figure D-4: Simulation values of the hardness-to-cohesion ratio, $H/c$. Level II - Mori-Tanaka + Mori-Tanaka - Perfectly adherent interfaces. [2/2]
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Figure D-5: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level II - Mori-Tanaka + Self-Consistent - Perfectly adherent interfaces. [1/2]
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Figure D-6: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level II - Mori-Tanaka + Self-Consistent - Perfectly adherent interfaces. [2/2]
Figure D-7: Simulation values of the hardness-to-cohesion ratio, $H/c_a$. Level II - Self-Consistent + Mori-Tanaka - Perfectly adherent interfaces. [1/2]
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Figure D-8: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level II - Self-Consistent + Mori-Tanaka - Perfectly adherent interfaces. [2/2]
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Figure D-9: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level II - Self-Consistent + Self-Consistent - Perfectly adherent interfaces. [1/2]
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Figure D-10: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level II - Self-Consistent + Self-Consistent - Perfectly adherent interfaces. [2/2]
\begin{tabular}{|l|c|c|c|c|c|c|c|c|c|c|}
\hline
$f_{inc}$ & \( \eta \backslash \alpha_s \) & 0.00 & 0.05 & 0.10 & 0.15 & 0.20 & 0.25 & 0.30 & 0.35 & 0.40 & 0.45 & 0.50 \\
\hline
0.05 & 0.00 & 4.76 & 5.35 & 6.04 & 6.81 & 7.67 & 8.67 & 9.86 & 11.29 & 13.07 & 15.35 & 18.50 \\
0.05 & 0.10 & 3.28 & 3.71 & 4.22 & 4.81 & 5.50 & 6.28 & 7.12 & 8.12 & 9.33 & 10.88 & 12.98 \\
0.05 & 0.20 & 2.27 & 2.57 & 2.93 & 3.37 & 3.86 & 4.46 & 5.15 & 5.91 & 6.74 & 7.78 & 9.14 \\
0.05 & 0.30 & 1.70 & 1.87 & 2.08 & 2.36 & 2.71 & 3.14 & 3.63 & 4.21 & 4.89 & 5.61 & 6.44 \\
0.05 & 0.40 & 1.30 & 1.41 & 1.54 & 1.70 & 1.92 & 2.18 & 2.54 & 2.95 & 3.43 & 4.00 & 4.61 \\
0.05 & 0.50 & 0.99 & 1.06 & 1.15 & 1.26 & 1.38 & 1.55 & 1.76 & 2.04 & 2.37 & 2.76 & 3.21 \\
0.05 & 0.60 & 0.74 & 0.79 & 0.84 & 0.91 & 0.99 & 1.09 & 1.22 & 1.37 & 1.59 & 1.85 & 2.16 \\
0.05 & 0.70 & 0.52 & 0.55 & 0.59 & 0.63 & 0.68 & 0.74 & 0.81 & 0.90 & 1.02 & 1.18 & 1.37 \\
0.05 & 0.80 & 0.32 & 0.34 & 0.36 & 0.38 & 0.41 & 0.44 & 0.48 & 0.53 & 0.60 & 0.68 & 0.79 \\
0.05 & 0.90 & 0.15 & 0.16 & 0.17 & 0.18 & 0.19 & 0.21 & 0.22 & 0.24 & 0.27 & 0.30 & 0.34 \\
\hline
0.10 & 0.00 & 4.75 & 5.34 & 6.03 & 6.79 & 7.65 & 8.66 & 9.86 & 11.32 & 13.14 & 15.49 & 18.79 \\
0.10 & 0.10 & 3.28 & 3.71 & 4.21 & 4.80 & 5.49 & 6.27 & 7.11 & 8.12 & 9.36 & 10.93 & 13.12 \\
0.10 & 0.20 & 2.28 & 2.57 & 2.94 & 3.36 & 3.86 & 4.45 & 5.14 & 5.90 & 6.75 & 7.78 & 9.19 \\
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0.10 & 0.50 & 0.99 & 1.07 & 1.15 & 1.26 & 1.39 & 1.55 & 1.76 & 2.04 & 2.37 & 2.75 & 3.21 \\
0.10 & 0.60 & 0.74 & 0.79 & 0.85 & 0.91 & 1.00 & 1.09 & 1.22 & 1.38 & 1.60 & 1.85 & 2.15 \\
0.10 & 0.70 & 0.52 & 0.55 & 0.59 & 0.63 & 0.68 & 0.74 & 0.82 & 0.91 & 1.03 & 1.18 & 1.37 \\
0.10 & 0.80 & 0.32 & 0.34 & 0.36 & 0.39 & 0.41 & 0.45 & 0.49 & 0.54 & 0.60 & 0.68 & 0.79 \\
0.10 & 0.90 & 0.15 & 0.16 & 0.17 & 0.18 & 0.19 & 0.21 & 0.22 & 0.24 & 0.27 & 0.30 & 0.34 \\
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0.15 & 0.00 & 4.73 & 5.32 & 6.00 & 6.76 & 7.62 & 8.63 & 9.84 & 11.31 & 13.16 & 15.58 & 19.01 \\
0.15 & 0.10 & 3.27 & 3.70 & 4.20 & 4.83 & 5.47 & 6.23 & 7.08 & 8.09 & 9.33 & 10.96 & 13.21 \\
0.15 & 0.20 & 2.28 & 2.58 & 2.94 & 3.36 & 3.85 & 4.43 & 5.12 & 5.87 & 6.71 & 7.77 & 9.21 \\
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\end{tabular}

Figure D-11: Simulation values of the hardness-to-cohesion ratio, \( H/c_s \). Level II - Mori-Tanaka + Mori-Tanaka - Slippery imperfect interfaces. [1/2]
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Figure D-12: Simulation values of the hardness-to-cohesion ratio, \( H/c_s \). Level II - Mori-Tanaka + Mori-Tanaka - Slippery imperfect interfaces. [2/2]
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Figure D-13: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level II - Mori-Tanaka + Self-Consistent - Slippery imperfect interfaces. [1/2]
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Figure D-14: Simulation values of the hardness-to-cohesion ratio, \( H/c_s \). Level II - Mori-Tanaka + Self-Consistent - Slippery imperfect interfaces. [2/2]
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Figure D-15: Simulation values of the hardness-to-cohesion ratio, \( H/c_s \). Level II - Self-Consistent + Mori-Tanaka - Slippery imperfect interfaces. [1/2]
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Figure D-16: Simulation values of the hardness-to-cohesion ratio, \( H/c_s \). Level II - Self-Consistent + Mori-Tanaka - Slippery imperfect interfaces. [2/2]
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Figure D-17: Simulation values of the hardness-to-cohesion ratio, $H/c_a$. Level II - Self-Consistent + Self-Consistent - Slippery imperfect interfaces. [1/2]
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Figure D-18: Simulation values of the hardness-to-cohesion ratio, $H/c_s$. Level II - Self-Consistent + Self-Consistent - Slippery imperfect interfaces. [2/2]
Bibliography


[41] A. Fritsch, L. Dormieux, C. Hellmich and J. Sanahuja. Micromechanics of crystal interfaces in polycrystalline solid phases of porous media: fundamentals and application to


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